现代物理基础丛书 86

# 开放量子系统的电子计数统计理论

薛海斌　著

科学出版社

现代物理基础丛书　86

# 开放量子系统的电子计数统计理论

薛海斌　著

科学出版社

北京

## 内 容 简 介

本书基于时间局域的量子主方程，介绍了开放量子系统的电子计数统计理论. 主要包括：密度矩阵理论、量子主方程、二阶非马尔可夫的电子计数统计理论、四阶非马尔可夫的电子计数统计理论和非马尔可夫电子计数统计理论的应用：顺序隧穿极限和共隧穿极限. 此外，书末 12 个附录给出了相关计算和推导过程中的关键细节.

本书读者对象为从事凝聚态物理相关研究方向的科研工作者、研究生，以及高年级本科生.

**图书在版编目（CIP）数据**

开放量子系统的电子计数统计理论/薛海斌著. —北京：科学出版社，2018. 12
(现代物理基础丛书)
ISBN 978-7-03-059914-8

Ⅰ. ①开… Ⅱ. ①薛… Ⅲ. ①量子统计力学-研究 Ⅳ. ①O414.2

中国版本图书馆 CIP 数据核字 (2018) 第 271501 号

责任编辑：周 涵 田轶静／责任校对：杨 然
责任印制：吴兆东／封面设计：陈 敬

**科学出版社** 出版
北京东黄城根北街 16 号
邮政编码：100717
http://www.sciencep.com

**北京建宏印刷有限公司** 印刷
科学出版社发行 各地新华书店经销
*
2018 年 12 月第 一 版 开本：720×1000 B5
2018 年 12 月第一次印刷 印张：14
字数：283 000

**定价：98.00 元**

(如有印装质量问题，我社负责调换)

# 前　　言

随着半导体微加工技术的进步和微纳器件实验设计水平的提高, 单分子器件已在实验上实现, 并且相关的实验技术也在快速发展. 对处于纳米尺度的开放量子系统, 电流涨落和电子关联将对其量子输运产生重要影响, 特别是, 电流噪声可以提供比平均电流和微分电导更多的关于该系统量子输运的微观机制信息. 因而, 从基础物理研究和实际应用的角度来看, 仅仅知道其电流和电导特性是不够的. 目前, 在实验上, 已在单量子点中实现高质量地实时测量电子通过单量子点的极微小电流, 并能够给出传输电子数目的前 15 阶瞬态累积矩及其有限频率的高阶累积矩. 因此, 电子通过受限小量子系统的全计数统计已成为量子输运领域的一个研究热点, 并且成为表征其量子输运性质的重要手段.

事实上, 在开放量子系统中, 电子的非平衡输运过程在本质上是一个量子统计随机过程, 因而, 在一段时间范围内该系统的传输电子数目是一个随机涨落量, 并且其分布函数完全依赖于该量子系统的内在属性. 若知道此分布函数, 就可以完全获得该系统的量子输运性质及其内部信息, 例如, 系统的内部能量标度及其内在动力学信息. 但是, 获取此分布函数是不可能完全做到的. 幸运的是, 起源于量子光学的光子计数统计理论在原则上可以计算出所有的零频电流关联, 即传输电子数目的所有阶累积矩. 由统计理论可知, 利用电流的各阶累积矩可以反推其分布函数, 例如, 前四阶累积矩分别对应于平均电流 (刻画传输电子数目分布峰的位置)、散粒噪声 (刻画传输电子数目分布峰的峰宽)、偏斜度 (刻画传输电子在其平均传输电子数附近分布的不对称性) 以及峭度 (刻画传输电子数目分布峰的峭度).

本书基于时间局域的量子主方程和瑞利–薛定谔微扰理论, 给出了开放量子系统在顺序隧穿和共隧穿极限下的电子计数统计理论, 尤其是, 以单量子点、串联耦合双量子点和 T 型双量子点三个系统为例, 给出了计算开放量子系统电子计数统计的计算流程, 以及相关的关键计算过程和细节, 其相关内容均来自作者的研究课题. 全书内容由 6 章和 12 个附录组成：第 1 章介绍了与量子主方程相关的密度矩阵理论; 第 2 章介绍并详细推导了费米黄金规则 ($T$ 矩阵)、率方程、马尔可夫量子主方程以及时间局域的非马尔可夫量子主方程, 并对推导过程中涉及的相关近似进行了讨论和说明; 第 3 章在顺序隧穿极限下给出了二阶时间局域的粒子数分辨量子主方程, 并基于此方程给出了两种计算开放量子系统电子全计数统计的方法; 第 4 章在共隧穿极限下给出了四阶时间局域的粒子数分辨量子主方程; 第 5 章以单量子点、串联耦合双量子点和 T 型双量子点三个系统为例, 讨论了非马尔可夫效应

和量子相干性对其电子计数统计的影响; 第 6 章以 T 型双量子点为例, 在顺序隧穿占主导地位的偏压区域内, 讨论了共隧穿过程和量子相干性对其电子计数统计的影响. 为方便读者, 在最后一部分的 12 个附录中, 给出了计算开放量子系统电子计数统计涉及的关键主值积分计算、一些关键公式推导的细节, 以及作为例子的量子点系统的条件性约化密度矩阵的矩阵元运动方程.

作者要特别感谢合作者以及课题组成员给予的支持与帮助. 另外, 还要感谢山西省高等学校优秀青年学术带头人支持计划 (2016)、山西省自然科学基金 (批准号：201601D011015), 以及国家自然科学基金 (批准号：11204203) 的资金支持. 由于开放量子系统的电子计数统计理论属于不断发展的前沿领域, 并且研究方法和内容在不断更新和发展, 书中难免有疏漏和不妥之处, 恳请读者批评指正, 作者邮箱: xuehaibin@tyut.edu.cn 和 xuehaibintyut@126.com.

薛海斌

2018 年 8 月于太原

# 目　　录

# 第 1 章　密度矩阵理论

一般情况下, 对于一个开放量子系统, 由于量子力学本身的物理特性或者统计物理性质, 其所处的状态不能用一个确定的量子态描述, 而是各个量子态以一定的概率出现. 本章介绍用密度算符描述量子系统微观状态的基本方法和相关理论[1-4].

## 1.1　纯态和混合态

在量子力学中, 微观粒子的状态可以用希尔伯特空间中的态矢量描述. 若一个量子系统的态可以用一个态矢量 $|\Psi\rangle$ 描写, 则这种态称为纯态. 此外, 几个纯态 $|\Psi_i\rangle$ 通过叠加得到的新的态

$$|\Psi\rangle = \sum_i c_i |\Psi_i\rangle, \tag{1.1}$$

也是纯态. 因而, 只要能够用希尔伯特空间中一个态矢量描写的状态都是纯态.

若一个量子系统的状态以一定的概率 $p_i$ 处于态矢量 $|\Psi_i\rangle\,(i=1,2,\cdots,N)$ 描写的态中, 即

$$\begin{cases} |\Psi_1\rangle : p_1 \\ |\Psi_2\rangle : p_2 \\ \qquad \vdots \\ |\Psi_N\rangle : p_N \end{cases}, \tag{1.2}$$

则上面这种无法用一个态矢量描写的状态, 称为混合态.

为说明纯态和混合态的不同, 这里考虑任意一个力学量 $A$ 的平均值. 在式 (1.1) 的纯态中, 力学量 $A$ 的平均值为

$$\begin{aligned} \langle A\rangle = \langle\Psi|\,A\,|\Psi\rangle &= \sum_{i,j} \langle\Psi_i|\,c_i^* A c_j\,|\Psi_j\rangle \\ &= \sum_{i=j} |c_i|^2 \langle\Psi_i|\,A\,|\Psi_i\rangle + \sum_{i\neq j} c_i^* c_j \langle\Psi_i|\,A\,|\Psi_j\rangle, \end{aligned} \tag{1.3}$$

而在式 (1.2) 的混合态中, 力学量 $A$ 的平均值为

$$\langle\langle A\rangle\rangle = \sum_i p_i \langle\Psi_i|\,A\,|\Psi_i\rangle. \tag{1.4}$$

由式 (1.3) 和式 (1.4) 可知, 在纯态中, 不同的两个态 $|\Psi_i\rangle$ 和 $|\Psi_j\rangle$ 之间发生干涉现象, 而在混合态情形下不发生干涉现象. 因此, 纯态是其各组分态的相干叠加, 而混合态是其各组分态的非相干叠加. 此外, 从式 (1.4) 还可以看出, 在一个混合态中求力学量的平均值应该分两步：第一, 对每个组分态求相应力学量的量子平均值; 第二, 求各组分态在混合态中出现概率的统计平均.

## 1.2 密 度 矩 阵

为更方便地描写混合态, 引入一个称之为密度算符的力学量来代替式 (1.2). 对于纯态, 其是混合态的一个特例, 即某一态矢量以 100% 的概率出现. 在态矢量 $|\Psi\rangle$ 描写的纯态中, 力学量 $A$ 的平均值为

$$\langle A\rangle = \langle\Psi| A |\Psi\rangle . \tag{1.5}$$

取态矢量 $|\Psi\rangle$ 的一组基矢 $\{|n\rangle\}$, 利用其完全性关系 $\sum\limits_n |n\rangle\langle n| = 1$, 将式 (1.5) 写为

$$\begin{aligned}\langle A\rangle &= \langle\Psi| A |\Psi\rangle = \sum_n \langle\Psi| |n\rangle \langle n| A |\Psi\rangle \\ &= \sum_n \langle n| A |\Psi\rangle \langle\Psi| |n\rangle = \sum_n \langle n| A\rho |n\rangle = \mathrm{tr}\,(A\rho)\,,\end{aligned} \tag{1.6}$$

其中

$$\rho = |\Psi\rangle\langle\Psi| . \tag{1.7}$$

式 (1.7) 中的 $\rho$ 称为密度算符, 其性质由态矢量 $|\Psi\rangle$ 决定. 这里需要注意的是, 构造密度算符时必须使用归一化的态矢量. 另外, 力学量 $A$ 在态矢量 $|\Psi\rangle$ 中取 $|n\rangle$ 的概率 $W_n$ 为

$$W_n = |\langle n| |\Psi\rangle|^2 = \langle n| |\Psi\rangle \langle\Psi| |n\rangle = \langle n| \rho |n\rangle\,, \tag{1.8}$$

式 (1.8) 中的概率即为密度算符在本征态 $|n\rangle$ 中的平均值. 因此, 对于一个纯态, 密度算符 $\rho$ 跟态矢量 $|\Psi\rangle$ 一样可以完全描述纯态的相关性质.

下面, 基于式 (1.4) 讨论混合态的密度算符. 为方便讨论, 同样选取 $\{|n\rangle\}$ 为基矢组, 相应地式 (1.4) 可以表示为

$$\begin{aligned}\langle\langle A\rangle\rangle &= \sum_n \sum_i p_i \langle\Psi_i| |n\rangle \langle n| A |\Psi_i\rangle \\ &= \sum_n \langle n| A \left[\sum_i |\Psi_i\rangle p_i \langle\Psi_i|\right] |n\rangle\end{aligned}$$

$$= \sum_n \langle n| A\rho |n\rangle = \mathrm{tr}\,(A\rho) = \mathrm{tr}\,(\rho A)\,, \tag{1.9}$$

其中

$$\rho = \sum_i |\Psi_i\rangle\, p_i\, \langle\Psi_i|. \tag{1.10}$$

式 (1.10) 中的 $\rho$ 称为混合态的密度算符. 此时, 在混合态中, 力学量 $A$ 的平均值可以表示为与纯态相同的形式, 即

$$\langle\langle A\rangle\rangle = \mathrm{tr}\,(A\rho)\,. \tag{1.11}$$

这里, 需要说明的是, 密度算符并不能给出混合态描写的粒子的位置分布概率, 但是, 在许多情况下, 采用统计平均的方法足以掌握系统的基本性质.

## 1.3　密度算符的性质

一般情况下, 一个混合态可以表示为

$$\rho = \sum_i |\Psi_i\rangle\, p_i\, \langle\Psi_i|, \tag{1.12}$$

其中 $\sum\limits_i p_i = 1$, $|\Psi_i\rangle\,(i = 1, 2, \cdots)$ 是构成混合态的纯态 (通常为系统哈密顿量的本征态), $p_i$ 是相应的权重. 由于态 $|\Psi_i\rangle$ 在混合态中出现的概率 $p_i$ 是实数, 因而

$$\rho^\dagger = \rho. \tag{1.13}$$

下面, 讨论密度算符的迹. 由完全性关系 $\sum\limits_n |n\rangle\langle n| = 1$ 可知

$$\begin{aligned}\mathrm{tr}\,(\rho) &= \sum_n \langle n| \sum_i |\Psi_i\rangle\, p_i\, \langle\Psi_i|\, |n\rangle = \sum_n \sum_i \langle n|\, |\Psi_i\rangle\, p_i\, \langle\Psi_i|\, |n\rangle \\ &= \sum_i p_i \langle\Psi_i| \sum_n |n\rangle\langle n|\, |\Psi_i\rangle = \sum_i p_i \langle\Psi_i|\, |\Psi_i\rangle = \sum_i p_i = 1,\end{aligned} \tag{1.14}$$

上式称为密度算符的归一化条件. 这里, 只利用了基矢组 $\{|n\rangle\}$ 的完全性关系, 并不需要基矢组中的态矢量两两相互正交. 另外, 由完全性关系还可得

$$\begin{aligned}\mathrm{tr}\left(\rho^2\right) &= \sum_n \langle n| \sum_i |\Psi_i\rangle\, p_i\, \langle\Psi_i| \sum_j |\Psi_j\rangle\, p_j\, \langle\Psi_j|\, |n\rangle \\ &= \sum_{i,j} \langle\Psi_i|\, |\Psi_j\rangle\, \langle\Psi_j| \sum_n |n\rangle\langle n|\, |\Psi_i\rangle\, p_i p_j\end{aligned}$$

$$
\begin{aligned}
&= \sum_{i,j} \langle \Psi_i | | \Psi_j \rangle \langle \Psi_j | | \Psi_i \rangle p_i p_j \\
&= \sum_i p_i \left[ \sum_j |\langle \Psi_i | | \Psi_j \rangle|^2 p_j \right],
\end{aligned} \tag{1.15}
$$

上式右边最后一项中的 $|\langle \Psi_i | | \Psi_j \rangle|^2$ 在 $i \neq j$(非纯态) 情形下, 其数值一定小于 1, 即

$$
\sum_j |\langle \Psi_i | | \Psi_j \rangle|^2 p_j < \sum_j p_j = 1, \tag{1.16}
$$

将式 (1.16) 代入式 (1.15), 并考虑到 $p_i < 1$, 可得

$$
\operatorname{tr}\left(\rho^2\right) < \sum_i p_i = 1. \tag{1.17}
$$

对于纯态的情形, 则有

$$
\begin{aligned}
\operatorname{tr}\left(\rho^2\right) &= \sum_n \langle n | | \Psi \rangle \langle \Psi | | \Psi \rangle \langle \Psi | | n \rangle \\
&= \sum_n \langle n | | \Psi \rangle \langle \Psi | | n \rangle \\
&= \langle \Psi | \sum_n | n \rangle \langle n | | \Psi \rangle = \langle \Psi | | \Psi \rangle = 1,
\end{aligned} \tag{1.18}
$$

由式 (1.17) 和式 (1.18) 可知, 密度算符具有如下性质:

$$
\operatorname{tr}\left(\rho^2\right) \begin{cases} = 1, & \text{纯态} \\ < 1, & \text{混合态} \end{cases}. \tag{1.19}
$$

上式可以作为微观状态是否为纯态的一个判据.

另外, 若构成混合态的各组分纯态相互正交, 即 $\langle \Psi_i | | \Psi_j \rangle = \delta_{i,j}$, 由密度算符的定义可知

$$
\rho | \Psi_j \rangle = \sum_i | \Psi_i \rangle p_i \langle \Psi_i | | \Psi_j \rangle = p_j | \Psi_j \rangle . \tag{1.20}
$$

上式表明, 密度算符的本征矢为构成混合态的各组分纯态的态矢量, 本征值为相应的组分态在混合态中的概率. 因此, 在构成混合态的各组分纯态相互正交时, 可以通过密度矩阵了解该混合态的状态分布.

## 1.4 密度算符的运动方程

一般情况下, 需要进一步研究量子态随时间的演化问题, 因此, 继续讨论密度算符在不同绘景中的演化方程. 在薛定谔绘景中, 密度算符是一个含时算符

$$
\rho(t) = \sum_i | \Psi_i(t) \rangle_{\mathrm{S}} \, p_i \, {}_{\mathrm{S}}\langle \Psi_i(t) |, \tag{1.21}
$$

其中 $p_i$ 不随时间变化 (平衡态情形). 对式 (1.21) 求关于时间的微分可得

$$\begin{aligned}
\mathrm{i}\hbar\frac{\partial\rho_{\mathrm{S}}(t)}{\partial t} &= \sum_i\left[\mathrm{i}\hbar\frac{\partial\left|\Psi_i(t)\right\rangle_{\mathrm{S}}}{\partial t}\right]p_i\ {}_{\mathrm{S}}\langle\Psi_i(t)| \\
&\quad -\sum_i\left|\Psi_i(t)\right\rangle_{\mathrm{S}}p_i\left[-\mathrm{i}\hbar\frac{\partial\ {}_{\mathrm{S}}\langle\Psi_i(t)|}{\partial t}\right] \\
&= \sum_i H\left|\Psi_i(t)\right\rangle_{\mathrm{S}}p_i\ {}_{\mathrm{S}}\langle\Psi_i(t)| - \sum_i\left|\Psi_i(t)\right\rangle_{\mathrm{S}}p_i\ {}_{\mathrm{S}}\langle\Psi_i(t)|\,H \\
&= H\rho_{\mathrm{S}}(t) - \rho_{\mathrm{S}}(t)H = [H,\rho_{\mathrm{S}}(t)],
\end{aligned} \tag{1.22}$$

上式即为密度算符的运动方程, 又称刘维尔方程. 这里, 需要注意区分密度算符的运动方程与海森伯绘景中描述力学量算符的运动方程之间的不同. 在能量表象中, 若设

$$H|n\rangle = E_n|n\rangle, \tag{1.23}$$

则刘维尔方程可以表示为

$$\begin{aligned}
\mathrm{i}\hbar\frac{\partial\langle n|\rho_{\mathrm{S}}(t)|m\rangle}{\partial t} &= \langle n|H\rho_{\mathrm{S}}(t)|m\rangle - \langle n|\rho_{\mathrm{S}}(t)H|m\rangle \\
&= (E_n - E_m)\langle n|\rho_{\mathrm{S}}(t)|m\rangle,
\end{aligned} \tag{1.24}$$

求解上式可得

$$\rho^{\mathrm{S}}_{n,m}(t) = \langle n|\rho_{\mathrm{S}}(t)|m\rangle = \rho^{\mathrm{S}}_{n,m}(0)\,\mathrm{e}^{-\mathrm{i}(E_n-E_m)t/\hbar}. \tag{1.25}$$

在海森伯绘景中, 态矢量不随时间变化, 力学量算符将随时间变化. 利用薛定谔绘景和海森伯绘景之间态矢量的变换关系

$$|\Psi_i(t)\rangle_{\mathrm{S}} = U(t,0)|\Psi_i\rangle_{\mathrm{H}}, \tag{1.26}$$

可得密度算符在薛定谔绘景和海森伯绘景之间的变换关系

$$\begin{aligned}
\rho_{\mathrm{S}}(t) &= |\Psi_i(t)\rangle_{\mathrm{S}}\,p_i\ {}_{\mathrm{S}}\langle\Psi_i(t)| \\
&= U(t,0)|\Psi_i\rangle_{\mathrm{H}}\,p_i\ {}_{\mathrm{H}}\langle\Psi_i|U^{-1}(t,0) = U(t,0)\rho_{\mathrm{H}}U^{-1}(t,0),
\end{aligned} \tag{1.27}$$

其中, $U(t,0)$ 为系统的时间演化算符.

现在, 讨论密度算符在相互作用绘景中的运动方程. 若系统的哈密顿量在薛定谔绘景中可以分解为

$$H_{\mathrm{S}} = H_0^{\mathrm{S}} + H_1^{\mathrm{S}}, \tag{1.28}$$

其中, $H_0^{\mathrm{S}}$ 为主要部分, 通常不含时且其性质已知; $H_1^{\mathrm{S}}$ 为微扰部分, 仅对整个系统有比较小的影响. 由相互作用绘景和薛定谔绘景之间态矢量的变换关系

$$|\Psi_i(t)\rangle_{\mathrm{S}} = \mathrm{e}^{-\mathrm{i}H_0^{\mathrm{S}}t/\hbar}|\Psi_i(t)\rangle_{\mathrm{I}}, \tag{1.29}$$

可得密度算符在相互作用绘景和薛定谔绘景之间的变换关系

$$\begin{aligned}\rho_{\mathrm{S}}(t) &= |\Psi_i(t)\rangle_{\mathrm{S}}\, p_i\; {}_{\mathrm{S}}\langle\Psi_i(t)| \\ &= \mathrm{e}^{-\mathrm{i}H_0^{\mathrm{S}}t/\hbar}\,|\Psi_i(t)\rangle_{\mathrm{I}}\, p_i\; {}_{\mathrm{I}}\langle\Psi_i(t)|\,\mathrm{e}^{\mathrm{i}H_0^{\mathrm{S}}t/\hbar} = \mathrm{e}^{-\mathrm{i}H_0^{\mathrm{S}}t/\hbar}\rho_{\mathrm{I}}(t)\,\mathrm{e}^{\mathrm{i}H_0^{\mathrm{S}}t/\hbar},\end{aligned} \tag{1.30}$$

即

$$\rho_{\mathrm{I}}(t) = \mathrm{e}^{\mathrm{i}H_0^{\mathrm{S}}t/\hbar}\rho_{\mathrm{S}}(t)\,\mathrm{e}^{-\mathrm{i}H_0^{\mathrm{S}}t/\hbar}, \tag{1.31}$$

对上式求关于时间的微分可得

$$\begin{aligned}&\mathrm{i}\hbar\frac{\partial\rho_{\mathrm{I}}(t)}{\partial t} \\ =&\,\mathrm{e}^{\mathrm{i}H_0^{\mathrm{S}}t/\hbar}\left(-H_0^{\mathrm{S}}\right)\rho_{\mathrm{S}}(t)\,\mathrm{e}^{-\mathrm{i}H_0^{\mathrm{S}}t/\hbar} \\ &+\mathrm{e}^{\mathrm{i}H_0^{\mathrm{S}}t/\hbar}\mathrm{i}\hbar\frac{\partial\rho_{\mathrm{S}}(t)}{\partial t}\mathrm{e}^{-\mathrm{i}H_0^{\mathrm{S}}t/\hbar} + \mathrm{e}^{\mathrm{i}H_0^{\mathrm{S}}t/\hbar}\rho_{\mathrm{S}}(t)\,H_0^{\mathrm{S}}\mathrm{e}^{-\mathrm{i}H_0^{\mathrm{S}}t/\hbar} \\ =&\,\mathrm{e}^{\mathrm{i}H_0^{\mathrm{S}}t/\hbar}\left[\rho_{\mathrm{S}}(t)\,H_0^{\mathrm{S}} - H_0^{\mathrm{S}}\rho_{\mathrm{S}}(t)\right]\mathrm{e}^{-\mathrm{i}H_0^{\mathrm{S}}t/\hbar} \\ &+\mathrm{e}^{\mathrm{i}H_0^{\mathrm{S}}t/\hbar}\left[H_{\mathrm{S}}\rho_{\mathrm{S}}(t) - \rho_{\mathrm{S}}(t)\,H_{\mathrm{S}}\right]\mathrm{e}^{-\mathrm{i}H_0^{\mathrm{S}}t/\hbar} \\ =&\,\mathrm{e}^{\mathrm{i}H_0^{\mathrm{S}}t/\hbar}\left[\left(H_{\mathrm{S}} - H_0^{\mathrm{S}}\right)\rho_{\mathrm{S}}(t) - \rho_{\mathrm{S}}(t)\left(H_{\mathrm{S}} - H_0^{\mathrm{S}}\right)\right]\mathrm{e}^{-\mathrm{i}H_0^{\mathrm{S}}t/\hbar} \\ =&\,\mathrm{e}^{\mathrm{i}H_0^{\mathrm{S}}t/\hbar}H_1^{\mathrm{S}}\mathrm{e}^{-\mathrm{i}H_0^{\mathrm{S}}t/\hbar}\mathrm{e}^{\mathrm{i}H_0^{\mathrm{S}}t/\hbar}\rho_{\mathrm{S}}(t)\,\mathrm{e}^{-\mathrm{i}H_0^{\mathrm{S}}t/\hbar} \\ &-\mathrm{e}^{\mathrm{i}H_0^{\mathrm{S}}t/\hbar}\rho_{\mathrm{S}}(t)\,\mathrm{e}^{-\mathrm{i}H_0^{\mathrm{S}}t/\hbar}\mathrm{e}^{\mathrm{i}H_0^{\mathrm{S}}t/\hbar}H_1^{\mathrm{S}}\mathrm{e}^{-\mathrm{i}H_0^{\mathrm{S}}t/\hbar},\end{aligned} \tag{1.32}$$

即

$$\mathrm{i}\hbar\frac{\partial\rho_{\mathrm{I}}(t)}{\partial t} = \left[H_1^{\mathrm{I}}(t)\,,\rho_{\mathrm{I}}(t)\right], \tag{1.33}$$

其中 $H_1^{\mathrm{I}}$ 和 $\rho_{\mathrm{I}}(t)$ 均为相互作用绘景中的算符, 即

$$H_1^{\mathrm{I}}(t) = \mathrm{e}^{\mathrm{i}H_0^{\mathrm{S}}t/\hbar}H_1^{\mathrm{S}}\mathrm{e}^{-\mathrm{i}H_0^{\mathrm{S}}t/\hbar}, \tag{1.34}$$

$$\rho_{\mathrm{I}}(t) = \mathrm{e}^{\mathrm{i}H_0^{\mathrm{S}}t/\hbar}\rho_{\mathrm{S}}(t)\,\mathrm{e}^{-\mathrm{i}H_0^{\mathrm{S}}t/\hbar}, \tag{1.35}$$

式 (1.33) 即为密度算符在相互作用绘景中的运动方程, 通过求解该方程, 即可确定在相互作用绘景中混合态随时间变化的动力学性质.

最后, 讨论基于密度矩阵在三种绘景中求力学量 $A$ 的平均值. 在薛定谔绘景中, 密度算符随时间变化, 力学量不随时间变化, 由式 (1.9) 可得

$$\begin{aligned}\frac{\partial\langle\langle A\rangle\rangle}{\partial t} &= \frac{\partial}{\partial t}\mathrm{tr}\left[\rho(t)\,A\right] = \mathrm{tr}\left[\frac{\partial\rho(t)}{\partial t}A\right] = \frac{1}{\mathrm{i}\hbar}\mathrm{tr}\left(\left[H,\rho\right]A\right) \\ &= \frac{1}{\mathrm{i}\hbar}\mathrm{tr}\left[H\rho A - \rho HA\right] = \frac{1}{\mathrm{i}\hbar}\mathrm{tr}\left[\rho AH - \rho HA\right] = \frac{1}{\mathrm{i}\hbar}\mathrm{tr}\left(\rho\left[A,H\right]\right),\end{aligned} \tag{1.36}$$

即

$$\mathrm{i}\hbar\frac{\partial\langle\langle A\rangle\rangle}{\partial t} = \langle[A,H]\rangle\,. \tag{1.37}$$

在海森伯绘景中, 密度算符不随时间变化, 而力学量随时间变化, 因而有

$$\begin{aligned}\frac{\partial\langle\langle A\rangle\rangle}{\partial t}&=\frac{\partial}{\partial t}\mathrm{tr}\left[\rho A\left(t\right)\right]=\mathrm{tr}\left[\rho\frac{\partial A\left(t\right)}{\partial t}\right]\\&=\frac{1}{\mathrm{i}\hbar}\mathrm{tr}\left(\rho\left[A,H\right]\right)=\frac{1}{\mathrm{i}\hbar}\left\langle\left[A,H\right]\right\rangle,\end{aligned}\tag{1.38}$$

由式 (1.37) 和式 (1.38) 可知, 力学量 $A$ 的平均值在薛定谔绘景和海森伯绘景中遵循相同的方程. 对于相互作用绘景, 密度算符和力学量均随时间变化, 因此有

$$\begin{aligned}\frac{\partial\langle\langle A\rangle\rangle}{\partial t}&=\frac{\partial}{\partial t}\mathrm{tr}\left[\rho\left(t\right)A\left(t\right)\right]=\mathrm{tr}\left[\frac{\partial\rho\left(t\right)}{\partial t}A\left(t\right)+\rho\left(t\right)\frac{\partial A\left(t\right)}{\partial t}\right]\\&=\frac{1}{\mathrm{i}\hbar}\mathrm{tr}\left(\left[H_1,\rho\right]A+\rho\left[A,H_0\right]\right)\\&=\frac{1}{\mathrm{i}\hbar}\mathrm{tr}\left[H_1\rho A+\rho AH_0-\rho H_1A-\rho H_0A\right]\\&=\frac{1}{\mathrm{i}\hbar}\mathrm{tr}\left[\rho A\left(H_0+H_1\right)-\rho\left(H_0+H_1\right)A\right]\\&=\frac{1}{\mathrm{i}\hbar}\mathrm{tr}\left(\rho\left[A,\left(H_0+H_1\right)\right]\right)=\frac{1}{\mathrm{i}\hbar}\mathrm{tr}\left(\rho\left[A,H\right]\right).\end{aligned}\tag{1.39}$$

因此, 在密度矩阵理论框架下, 力学量 $A$ 的平均值在三种绘景中遵循相同的方程.

## 1.5　相干叠加与非相干叠加

对于一个量子系统, 假设其密度矩阵可以用态矢量 $\{|\Psi_i\rangle\}$ 的表象描述. 若在 $\{|\Psi_i\rangle\}$ 表象中, 其密度矩阵 $\rho$ 含有非对角元, 则称该系统是态矢量 $|\Psi_i\rangle$ 的相干叠加; 特别的, 若系统是一个纯态, 则称之为完全相干叠加. 反之, 若系统的密度矩阵 $\rho$ 仅有对角元, 则称该系统是态矢量 $|\Psi_i\rangle$ 的非相干叠加. 事实上, 区分 “完全相干” 和 “相干” 没有特别重要的意义, 并且在文献中 “相干” 一词通常使用于上面的两种情况. 因此, 在本书中, 遵循上述传统, 使用 “相干” 一词时, 不再考虑系统是否处于纯态或者混合态.

由上面分析可知, “相干叠加” 的概念取决于量子系统密度矩阵的表象选择. 例如, 式 (1.12) 描述的混合态是态矢量 $|\Psi_i\rangle$ 的非相干叠加. 但是, 在满足完全性条件

$$\sum_n\left|\phi_n\right\rangle\left\langle\phi_n\right|=1,\tag{1.40}$$

和正交性

$$\left\langle\phi_n\right|\left|\phi_m\right\rangle=\delta_{n,m},\tag{1.41}$$

的态矢量 $\{|\phi_n\rangle\}$ 表象中, 式 (1.12) 描述的混合态可以表示为

$$
\begin{aligned}
\rho &= \sum_i |\Psi_i\rangle\, p_i\, \langle\Psi_i| \\
&= \sum_i \sum_{n,m} c_{i,n}\, |\phi_n\rangle p_i\, \langle\phi_m| c^*_{i,m} = \sum_{i,n,m} p_i c_{i,n} c^*_{i,m}\, |\phi_n\rangle\, \langle\phi_m|.
\end{aligned} \tag{1.42}
$$

考虑上式中的密度算符在态 $|\phi_k\rangle$ 和 $\langle\phi_j|$ 中的矩阵元, 并考虑其正交性条件可得

$$
\begin{aligned}
\langle\phi_j|\, \rho\, |\phi_k\rangle &= \sum_{i,n,m} p_i\, \langle\phi_j|\, c_{i,n} c^*_{i,m}\, |\phi_n\rangle\, \langle\phi_m|\, |\phi_k\rangle \\
&= \sum_{i,n,m} p_i c_{i,n} c^*_{i,m} \delta_{j,n} \delta_{m,k} = \sum_i p_i c_{i,j} c^*_{i,k}.
\end{aligned} \tag{1.43}
$$

由式 (1.43) 可知, 式 (1.12) 描述的混合态也可以表示为态矢量 $|\phi_n\rangle$ 的相干叠加. 因此, 在密度矩阵理论中, 密度矩阵的非对角元刻画了基矢组中不同态矢量之间的相干性 [3]. 在本书后面的章节中, 重点讨论量子系统约化密度矩阵的非对角元, 即量子相干性对其非马尔可夫电子计数统计特性的影响 [5,6].

## 参 考 文 献

[1] 徐在新. 高等量子力学. 上海：华东师范大学出版社, 1994：2-13, 80-94.

[2] 喀兴林. 高等量子力学. 北京：高等教育出版社, 2001：42-51, 155-168, 192-205.

[3] Blum K. Density Matrix Theory and Applications. 3rd ed. Dordrecht: Springer, 2012: Chap. 1 and Chap. 2.

[4] Schaller G. Open Quantum Systems Far from Equilibrium. Dordrecht: Springer, 2014: 10-16.

[5] Xue H B, Jiao H J, Liang J Q, et al. Non-Markovian full counting statistics in quantum dot molecules. Sci. Rep., 2015, 5: 8978.

[6] Xue H B, Liang J Q, Liu W M. Non-Markovian full counting statistics of cotunneling assisted sequential tunneling in a side-coupled double quantum dot system. Physica E: Low-dimensional Systems and Nanostructures, 2019, 109: 39-51.

# 第 2 章　量子主方程

本章主要研究开放量子系统电子输运性质时的几种量子主方程方法, 并讨论相关方法的适用范围及其相关近似. 最后, 讨论这些方法在何种条件下可以等效的问题.

为方便讨论, 考虑一个如图 2.1 所示的典型开放量子系统, 即一个人们感兴趣的量子系统与两个电子库弱耦合, 整个系统的哈密顿量可以表示为

$$H = H_{\mathrm{QS}}\left(d_\mu^\dagger, d_\mu\right) + \sum_{\alpha=\mathrm{L,R}} \sum_{\boldsymbol{k}\sigma} \varepsilon_{\alpha\boldsymbol{k}\sigma} a_{\alpha\boldsymbol{k}\sigma}^\dagger a_{\alpha\boldsymbol{k}\sigma} + \sum_{\alpha=\mathrm{L,R}} \sum_{\mu\boldsymbol{k}\sigma} \left(t_{\alpha\mu\boldsymbol{k}\sigma} d_\mu^\dagger a_{\alpha\boldsymbol{k}\sigma} + \mathrm{H.c.}\right), \tag{2.1}$$

其中, $H_{\mathrm{QS}}\left(d_\mu^\dagger, d_\mu\right)$ 是所研究量子系统的哈密顿量, $d_\mu^\dagger(d_\mu)$ 是其电子的产生 (湮灭) 算符, $\mu$ 是其态指标 (如系统能级、电子自旋等). 第二项为电子库, 即源极和漏极的哈密顿量 $H_{\mathrm{leads}}$, 其中 $a_{\alpha\boldsymbol{k}\sigma}^\dagger(a_{\alpha\boldsymbol{k}\sigma})$ 表示在 $\alpha$ 电极上产生 (湮灭) 一个动量为 $\boldsymbol{k}$, 自旋为 $\sigma$ 的电子. 最后一项描述了所研究的量子系统与电极的隧穿耦合哈密顿量 $H_{\mathrm{T}}$.

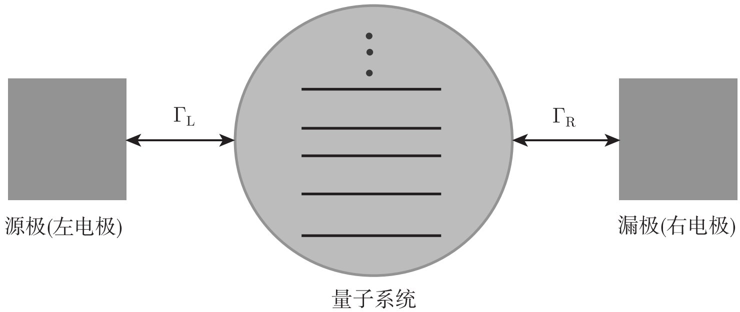


图 2.1　一个量子系统与两个电子库 (电极) 耦合可以形成一个典型的开放量子系统. 这里, 量子系统包含单分子、耦合量子点等低维受限量子系统和微纳系统. 鉴于量子主方程的微扰近似, 通常考虑量子系统与两个电子库或者源极、漏极的弱耦合情形. 此时, 量子主方程在二阶近似下的顺序隧穿和四阶近似下的共隧穿可以很好地描述此类电子隧穿过程

## 2.1　$T$ 矩阵和费米黄金规则

为方便推导系统密度矩阵的含时演化方程, 将式 (2.1) 重新写成如下形式：

$$H = H_0 + H_{\mathrm{T}}, \tag{2.2}$$

其中

$$H_0 = H_{\mathrm{QS}} + H_{\mathrm{leads}}, \tag{2.3}$$

$$H_{\mathrm{T}} = \sum_{\alpha=\mathrm{L,R}} \sum_{\mu \boldsymbol{k} \sigma} \left( t_{\alpha\mu\boldsymbol{k}\sigma} d_{\mu}^{\dagger} a_{\alpha\boldsymbol{k}\sigma} + \mathrm{H.c.} \right). \tag{2.4}$$

这里, 将量子系统与电极的隧穿耦合哈密顿量 $H_{\mathrm{T}}$ 看作微扰项. 在相互作用绘景中, 整个系统的哈密顿量 $H$ 对应的波函数满足

$$\mathrm{i}\hbar \frac{\partial}{\partial t} \left| \Psi(t) \right\rangle_{\mathrm{I}} = H_{\mathrm{T,I}}(t) \left| \Psi(t) \right\rangle_{\mathrm{I}}, \tag{2.5}$$

$$\left| \Psi(t) \right\rangle_{\mathrm{I}} = U_{\mathrm{I}}(t, t_0) \left| \Psi(t_0) \right\rangle_{\mathrm{I}}, \tag{2.6}$$

其中 $U_{\mathrm{I}}(t, t_0)$ 为相互作用绘景中的时间演化算符. 利用波函数在薛定谔绘景和相互作用绘景之间的变换关系可得

$$\left| \Psi(t) \right\rangle_{\mathrm{I}} = \mathrm{e}^{\mathrm{i}H_0 t/\hbar} \left| \Psi(t) \right\rangle_{\mathrm{S}} = \mathrm{e}^{\mathrm{i}H_0 t/\hbar} \mathrm{e}^{-\mathrm{i}Ht/\hbar} \left| \Psi(t=0) \right\rangle, \tag{2.7}$$

将上式代入式 (2.6), 并考虑到 $\left| \Psi(t_0) \right\rangle_{\mathrm{I}} = \mathrm{e}^{\mathrm{i}H_0 t_0/\hbar} \mathrm{e}^{-\mathrm{i}Ht_0/\hbar} \left| \Psi(t=0) \right\rangle$ 可得

$$\mathrm{e}^{\mathrm{i}H_0 t/\hbar} \mathrm{e}^{-\mathrm{i}Ht/\hbar} \left| \Psi(t=0) \right\rangle = U_{\mathrm{I}}(t, t_0) \mathrm{e}^{\mathrm{i}H_0 t_0/\hbar} \mathrm{e}^{-\mathrm{i}Ht_0/\hbar} \left| \Psi(t=0) \right\rangle, \tag{2.8}$$

即

$$U_{\mathrm{I}}(t, t_0) = \mathrm{e}^{\mathrm{i}H_0 t/\hbar} \mathrm{e}^{-\mathrm{i}H(t-t_0)/\hbar} \mathrm{e}^{-\mathrm{i}H_0 t_0/\hbar}. \tag{2.9}$$

对式 (2.9) 求关于时间的微分可得

$$\begin{aligned} &\mathrm{i}\hbar \frac{\partial}{\partial t} U_{\mathrm{I}}(t, t_0) \\ =& -\mathrm{e}^{\mathrm{i}H_0 t/\hbar} H_0 \mathrm{e}^{-\mathrm{i}H(t-t_0)/\hbar} \mathrm{e}^{-\mathrm{i}H_0 t_0/\hbar} + \mathrm{e}^{\mathrm{i}H_0 t/\hbar} H \mathrm{e}^{-\mathrm{i}H(t-t_0)/\hbar} \mathrm{e}^{-\mathrm{i}H_0 t_0/\hbar} \\ =& \mathrm{e}^{\mathrm{i}H_0 t/\hbar} (H - H_0) \mathrm{e}^{-\mathrm{i}H_0 t/\hbar} \mathrm{e}^{\mathrm{i}H_0 t/\hbar} \mathrm{e}^{-\mathrm{i}H(t-t_0)/\hbar} \mathrm{e}^{-\mathrm{i}H_0 t_0/\hbar}, \end{aligned} \tag{2.10}$$

即

$$\mathrm{i}\hbar \frac{\partial}{\partial t} U_{\mathrm{I}}(t, t_0) = H_{\mathrm{T,I}}(t) U_{\mathrm{I}}(t, t_0), \tag{2.11}$$

上式的形式解可以写为

$$\begin{aligned} U_{\mathrm{I}}(t, t_0) &= \mathrm{e}^{\frac{1}{\mathrm{i}\hbar} \int_{t_0}^{t} H_{\mathrm{T,I}}(t') \mathrm{d}t'} \\ &= 1 + \frac{1}{\mathrm{i}\hbar} \int_{t_0}^{t} H_{\mathrm{T,I}}(t_1) \mathrm{d}t_1 + \frac{1}{(\mathrm{i}\hbar)^2} \int_{t_0}^{t} H_{\mathrm{T,I}}(t_1) \mathrm{d}t_1 \int_{t_0}^{t_1} H_{\mathrm{T,I}}(t_2) \mathrm{d}t_2 + \cdots \end{aligned} \tag{2.12}$$

对于式 (2.2) 描述的量子系统, 在微扰项 $H_{\mathrm{T}}$ 未打开之前, 该系统处于能量为 $E_i$ 的量子态 $|i\rangle$. 在 $t_0$ 时刻, 将微扰项 $H_{\mathrm{T}}$ 打开, 此时, 系统在 $t$ 时刻处于能量为 $E_f$ 的量子态 $|f\rangle$ 的概率为

$$P_{i \to f} = \left| \langle f | \, | i(t) \rangle \right|^2, \tag{2.13}$$

对式 (2.13) 求关于时间的微分可得, 初态 $|i\rangle$ 到末态 $|f\rangle$ 的跃迁概率

$$\Gamma_{i\to f}=\frac{\mathrm{d}P_{i\to f}}{\mathrm{d}t}. \tag{2.14}$$

在薛定谔绘景中, 态矢量的时间演化可以表示为

$$|i\left(t\right)\rangle=U\left(t,t_0\right)|i\rangle=\mathrm{e}^{-\mathrm{i}H(t-t_0)/\hbar}\,|i\rangle=\mathrm{e}^{-\mathrm{i}H_0t/\hbar}U_{\mathrm{I}}\left(t,t_0\right)\mathrm{e}^{\mathrm{i}H_0t_0/\hbar}\,|i\rangle\,, \tag{2.15}$$

因此, 在 $t$ 时刻, 初态 $|i\rangle$ 到末态 $|f\rangle$ 的跃迁概率幅为

$$\begin{aligned}
&\langle f|\,|i\left(t\right)\rangle\\
&=\langle f|\,\mathrm{e}^{-\mathrm{i}H_0t/\hbar}U_{\mathrm{I}}\left(t,t_0\right)\mathrm{e}^{\mathrm{i}H_0t_0/\hbar}\,|i\rangle=\mathrm{e}^{-\mathrm{i}E_ft/\hbar}\mathrm{e}^{\mathrm{i}E_it_0/\hbar}\,\langle f|\,U_{\mathrm{I}}\left(t,t_0\right)|i\rangle\\
&=\mathrm{e}^{-\mathrm{i}E_ft/\hbar}\mathrm{e}^{\mathrm{i}E_it_0/\hbar}\,\langle f|\,\frac{1}{\mathrm{i}\hbar}\int_{t_0}^{t}H_{\mathrm{T,I}}\left(t_1\right)\mathrm{d}t_1\\
&\quad+\frac{1}{\left(\mathrm{i}\hbar\right)^2}\int_{t_0}^{t}H_{\mathrm{T,I}}\left(t_1\right)\mathrm{d}t_1\int_{t_0}^{t_1}H_{\mathrm{T,I}}\left(t_2\right)\mathrm{d}t_2+\cdots|i\rangle\,.
\end{aligned} \tag{2.16}$$

这里, 需要讨论量子系统的微扰项如何打开的问题 [1]. 由于具体的跃迁过程与本章讨论的问题不相关, 为方便问题讨论和计算, 通常将式 (2.2) 中的微扰项写为

$$H=H_0+H_{\mathrm{T}}\mathrm{e}^{\eta t}, \tag{2.17}$$

即假设微扰项缓慢打开. 事实上, 在许多问题中, 散射时间通常发生在微扰打开的时刻 $t_0$ 和测量时间 $t$ 之间, 因此, 需要微扰打开的时间 $\eta^{-1}$ 要与相互作用的时间 $t-t_0$ 很好地分离, 即 $(t-t_0)\gg\eta^{-1}$. 为了保持 $t$ 为有限值, 通常选取 $\eta\to0$, 此时 $t_0\to-\infty$. 一个实现上述条件的可行办法是, 引入一个费米函数 $f\left(t\right)=\left[1+\mathrm{e}^{-\eta(t-t_0)}\right]^{-1}$, 其表征了在 $t_0$ 时刻微扰在特征时间间隔 $\eta^{-1}$ 内打开. 相应地, 式 (2.16) 中的任意一项 $H_{\mathrm{T,I}}^{(n)}$ 可展开为

$$\begin{aligned}
&H_{\mathrm{T,I}}^{(n)}\\
&=\frac{1}{\left(\mathrm{i}\hbar\right)^n}\int_{-\infty}^{t}H_{\mathrm{T,I}}\left(t_1\right)f\left(t_1\right)\mathrm{d}t_1\cdots\\
&\quad\times\int_{-\infty}^{t_{i-1}}H_{\mathrm{T,I}}\left(t_i\right)f\left(t_i\right)\mathrm{d}t_i\cdots\int_{-\infty}^{t_{n-1}}H_{\mathrm{T,I}}\left(t_n\right)f\left(t_n\right)\mathrm{d}t_n,
\end{aligned} \tag{2.18}$$

在上式中, 当 $f\left(t_n\right)$ 打开后, 由于其余因子 $f\left(t_i\right)$ 的时间变量 $t_i>t_n$, 并且在适当的近似下有 $(t-t_0)\gg\eta^{-1}$, 因而, 当 $i\neq n$ 时, $f\left(t_i\right)=1$. 此时, 式 (2.18) 中仅含有一个微扰打开的时间. 当 $t_0\to-\infty$ 时, 可将 $f\left(t\right)$ 写成指数函数, 即 $f\left(t\right)\simeq\mathrm{e}^{\eta t}$. 利用此近似和式 (2.16), 可得

$$|\langle f|\,|i\left(t\right)\rangle|=\left|\,\langle f|\sum_n\frac{1}{\left(\mathrm{i}\hbar\right)^n}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\cdots\right.$$

$$\times\int_{-\infty}^{t_{n-1}}\mathrm{d}t_n H_{\mathrm{T,I}}(t_1)H_{\mathrm{T,I}}(t_2)\cdots H_{\mathrm{T,I}}(t_n)\,\mathrm{e}^{\eta t_n}\left|i\right\rangle\Bigg|. \tag{2.19}$$

当 $n=1$ 时, 式 (2.19) 可简化为

$$\begin{aligned}
&\left|\left\langle f\right|\left|i(t)\right\rangle\right|_{n=1}\\
=&\left|\frac{1}{\mathrm{i}\hbar}\left\langle f\right|\int_{-\infty}^{t}\mathrm{d}t_1 H_{\mathrm{T,I}}(t_1)\mathrm{e}^{\eta t_1}\left|i\right\rangle\right|=\frac{1}{\mathrm{i}\hbar}\left|\left\langle f\right|\int_{-\infty}^{t}\mathrm{d}t_1\mathrm{e}^{\mathrm{i}H_0t_1/\hbar}H_{\mathrm{T}}\mathrm{e}^{-\mathrm{i}H_0t_1/\hbar}\mathrm{e}^{\eta t_1}\left|i\right\rangle\right|\\
=&\left|\frac{1}{\mathrm{i}\hbar}\int_{-\infty}^{t}\mathrm{d}t_1\mathrm{e}^{\mathrm{i}(E_f-E_i-\mathrm{i}\eta\hbar)t_1/\hbar}\left\langle f\right|H_{\mathrm{T}}\left|i\right\rangle\right|=\left|-\frac{\left\langle f\right|H_{\mathrm{T}}\left|i\right\rangle}{E_f-E_i-\mathrm{i}\eta\hbar}\,\mathrm{e}^{\mathrm{i}(E_f-E_i-\mathrm{i}\eta\hbar)t_1/\hbar}\Big|_{-\infty}^{t}\right|\\
=&\left|\frac{\mathrm{e}^{\mathrm{i}(E_f-E_i-\mathrm{i}\eta\hbar)t/\hbar}\left\langle f\right|H_{\mathrm{T}}\left|i\right\rangle}{E_i-E_f+\mathrm{i}\eta\hbar}\right|=\left|\frac{\mathrm{e}^{\eta t}\left\langle f\right|H_{\mathrm{T}}\left|i\right\rangle}{E_i-E_f+\mathrm{i}\eta\hbar}\right|,
\end{aligned}\tag{2.20}$$

相应地式 (2.14) 可以表示为

$$\begin{aligned}
\Gamma_{i\to f}\big|_{n=1}=&\left.\frac{\mathrm{d}\left|\left\langle f\right|\left|i(t)\right\rangle\right|^2}{\mathrm{d}t}\right|_{n=1}=2\lim_{\eta\to 0}\frac{\eta\mathrm{e}^{2\eta t}}{(E_i-E_f)^2+(\eta\hbar)^2}\left|\left\langle f\right|H_{\mathrm{T}}\left|i\right\rangle\right|^2\\
=&\frac{2}{\hbar}\lim_{\eta\hbar\to 0}\frac{\eta\hbar}{(E_i-E_f)^2+(\eta\hbar)^2}\mathrm{e}^{2t\eta\hbar/\hbar}\left|\left\langle f\right|H_{\mathrm{T}}\left|i\right\rangle\right|^2\\
=&\frac{2\pi}{\hbar}\left|\left\langle f\right|H_{\mathrm{T}}\left|i\right\rangle\right|^2\delta(E_i-E_f),
\end{aligned}\tag{2.21}$$

其中, 上式计算中利用了 $\delta$ 函数的性质

$$\lim_{\eta\to 0}\frac{\eta}{x^2+\eta^2}=\pi\delta(x). \tag{2.22}$$

当 $n=2$ 时, 式 (2.19) 可简化为

$$\begin{aligned}
&\left|\left\langle f\right|\left|i(t)\right\rangle\right|_{n=2}\\
=&\left|\left\langle f\right|\frac{1}{(\mathrm{i}\hbar)^2}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2 H_{\mathrm{T,I}}(t_1)H_{\mathrm{T,I}}(t_2)\,\mathrm{e}^{\eta t_2}\left|i\right\rangle\right|\\
=&\left|\frac{1}{(\mathrm{i}\hbar)^2}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\sum_l\left\langle f\right|\mathrm{e}^{\mathrm{i}H_0t_1/\hbar}H_{\mathrm{T}}\mathrm{e}^{-\mathrm{i}H_0t_1/\hbar}\left|l\right\rangle\left\langle l\right|\mathrm{e}^{\mathrm{i}H_0t_2/\hbar}H_{\mathrm{T}}\mathrm{e}^{-\mathrm{i}H_0t_2/\hbar}\mathrm{e}^{\eta t_2}\left|i\right\rangle\right|\\
=&\left|\frac{1}{(\mathrm{i}\hbar)^2}\sum_l\int_{-\infty}^{t}\mathrm{e}^{\mathrm{i}(E_f-E_l)t_1/\hbar}\mathrm{d}t_1\left\langle f\right|H_{\mathrm{T}}\left|l\right\rangle\int_{-\infty}^{t_1}\mathrm{e}^{\mathrm{i}(E_l-E_i-\mathrm{i}\eta\hbar)t_2/\hbar}\mathrm{d}t_2\left\langle l\right|H_{\mathrm{T}}\left|i\right\rangle\right|\\
=&\left|\frac{1}{\mathrm{i}\hbar}\sum_l\int_{-\infty}^{t}\mathrm{e}^{\mathrm{i}(E_f-E_l)t_1/\hbar}\mathrm{d}t_1\left\langle f\right|H_{\mathrm{T}}\left|l\right\rangle\frac{\mathrm{e}^{\mathrm{i}(E_l-E_i-\mathrm{i}\eta\hbar)t_2/\hbar}\Big|_{-\infty}^{t_1}}{(E_i-E_l+\mathrm{i}\eta\hbar)}\left\langle l\right|H_{\mathrm{T}}\left|i\right\rangle\right|\\
=&\left|\sum_l\frac{1}{E_i-E_f+\mathrm{i}\eta\hbar}\,\mathrm{e}^{\mathrm{i}(E_f-E_i-\mathrm{i}\eta\hbar)t_1/\hbar}\Big|_{-\infty}^{t}\left\langle f\right|H_{\mathrm{T}}\left|l\right\rangle\frac{1}{E_i-E_l+\mathrm{i}\eta\hbar}\left\langle l\right|H_{\mathrm{T}}\left|i\right\rangle\right|
\end{aligned}$$

$$= \left| \frac{\mathrm{e}^{\mathrm{i}(E_f - E_i - \mathrm{i}\eta\hbar)t/\hbar}}{E_i - E_f + \mathrm{i}\eta\hbar} \langle f | H_\mathrm{T} \sum_l \frac{1}{E_i - E_l + \mathrm{i}\eta\hbar} |l\rangle \langle l | H_\mathrm{T} |i\rangle \right|, \tag{2.23}$$

因而, 相应地式 (2.14) 可以表示为

$$\begin{aligned} \Gamma_{i\to f}\big|_{n=2} &= \left.\frac{\mathrm{d}\left|\langle f| |i(t)\rangle\right|^2}{\mathrm{d}t}\right|_{n=2} \\ &= \frac{2\eta \mathrm{e}^{2\eta t}}{(E_i - E_f)^2 + (\eta\hbar)^2} \left| \langle f | H_\mathrm{T} \sum_l \frac{1}{E_i - H_0 + \mathrm{i}\eta\hbar} |l\rangle \langle l | H_\mathrm{T} |i\rangle \right|^2 \\ &= \frac{2}{\hbar} \lim_{\eta\hbar\to 0} \frac{\eta\hbar \mathrm{e}^{2t\eta\hbar/\hbar}}{(E_i - E_f)^2 + (\eta\hbar)^2} \left| \langle f | H_\mathrm{T} \frac{1}{E_i - H_0 + \mathrm{i}\eta\hbar} H_\mathrm{T} |i\rangle \right|^2 \\ &= \frac{2\pi}{\hbar} \left| \langle f | H_\mathrm{T} \frac{1}{E_i - H_0 + \mathrm{i}\eta} H_\mathrm{T} |i\rangle \right|^2 \delta(E_i - E_f). \end{aligned} \tag{2.24}$$

以此类推, 可以证明式 (2.14) 最后可以表示为

$$\Gamma_{i\to f} = \frac{2\pi}{\hbar} \left|\langle f| T |i\rangle\right|^2 \delta(E_i - E_f), \tag{2.25}$$

其中 $T$ 矩阵由下面的表达式自洽给出:

$$T = H_\mathrm{T} + H_\mathrm{T} \frac{1}{E_i - H_0 + \mathrm{i}\eta} T. \tag{2.26}$$

式 (2.26) 即为文献中通常所说的费米黄金规则.

## 2.2 率 方 程

在一个典型的量子输运问题中, 量子系统的电子输运性质是人们关注的重要问题, 其大小依赖于该系统不同能级的占据概率. 若该量子系统的哈密顿量 $H_\mathrm{QS}(d_\mu^\dagger, d_\mu)$ 的本征值和本征态满足

$$H_\mathrm{QS}\left(d_\mu^\dagger, d_\mu\right) |n\rangle = \varepsilon_n |n\rangle, \tag{2.27}$$

其中, $n = 1, 2, \cdots$. 此时, 量子系统在 $|n\rangle$ 态的概率随时间的演化可由率方程描述 [2,3]

$$\frac{\mathrm{d}P_n}{\mathrm{d}t} = \sum_{m\neq n} (R_{m\to n} P_m - R_{n\to m} P_n), \tag{2.28}$$

其中 $P_n = \langle n| \rho_\mathrm{QS} |n\rangle$. 这里, $R_{m\to n}$ 表示当量子系统与电子库耦合时其量子态从 $|m\rangle$ 到 $|n\rangle$ 的跃迁概率, 其数值可通过费米黄金规则, 即通过式 (2.25) 计算得出.

当量子系统与电子库弱耦合时, 式 (2.25) 中的一阶项就可以描述电子通过量子系统的隧穿过程. 设开放量子系统的初态和末态由电子库和量子系统的能量本征态组成, 即

$$|i\rangle = |\nu_{\mathrm{L}}, \nu_{\mathrm{R}}\rangle\, |n\rangle\,, \quad E_i = \varepsilon_n, \tag{2.29}$$

$$|f\rangle = \begin{cases} a_{\alpha\boldsymbol{k}\sigma}\, |\nu_{\mathrm{L}}, \nu_{\mathrm{R}}\rangle\, |m\rangle\,, & E_f = \varepsilon_m - \varepsilon_{\alpha\boldsymbol{k}\sigma} \\ a^{\dagger}_{\alpha\boldsymbol{k}\sigma}\, |\nu_{\mathrm{L}}, \nu_{\mathrm{R}}\rangle\, |m\rangle\,, & E_f = \varepsilon_m + \varepsilon_{\alpha\boldsymbol{k}\sigma} \end{cases}. \tag{2.30}$$

由式 (2.4) 和式 (2.25) 可得 $R_{n\to m}$ 中不为零的项为

$$\begin{aligned} &R_{n\to m} \\ =&\frac{2\pi}{\hbar}\sum_{\alpha\mu\boldsymbol{k}\sigma}\sum_{\nu_{\mathrm{L}},\nu_{\mathrm{R}}} W_{\nu_{\mathrm{L}},\nu_{\mathrm{R}}} \left|\langle m|\,\langle \nu_{\mathrm{R}}, \nu_{\mathrm{L}}|\, a^{\dagger}_{\alpha\boldsymbol{k}\sigma} t_{\alpha\mu\boldsymbol{k}\sigma} d^{\dagger}_{\mu} a_{\alpha\boldsymbol{k}\sigma}\, |\nu_{\mathrm{L}}, \nu_{\mathrm{R}}\rangle\, |n\rangle\right|^2 \delta\left(E_i - E_f\right) \\ &+ \frac{2\pi}{\hbar}\sum_{\alpha\mu\boldsymbol{k}\sigma}\sum_{\nu_{\mathrm{L}},\nu_{\mathrm{R}}} W_{\nu_{\mathrm{L}},\nu_{\mathrm{R}}} \left|\langle m|\,\langle \nu_{\mathrm{R}}, \nu_{\mathrm{L}}|\, a_{\alpha\boldsymbol{k}\sigma} t^{*}_{\alpha\mu\boldsymbol{k}\sigma} a^{\dagger}_{\alpha\boldsymbol{k}\sigma} d_{\mu}\, |\nu_{\mathrm{L}}, \nu_{\mathrm{R}}\rangle\, |n\rangle\right|^2 \delta\left(E_i - E_f\right), \end{aligned} \tag{2.31}$$

将式 (2.31) 中的模方项展开可得

$$\begin{aligned} R_{n\to m} =& \frac{2\pi}{\hbar}\sum_{\alpha\mu\boldsymbol{k}\sigma}\sum_{\nu_{\mathrm{L}},\nu_{\mathrm{R}}} \left|t_{\alpha\mu\boldsymbol{k}\sigma}\right|^2 W_{\nu_{\mathrm{L}},\nu_{\mathrm{R}}} \langle \nu_{\mathrm{R}}, \nu_{\mathrm{L}}|\, a^{\dagger}_{\alpha\boldsymbol{k}\sigma} a_{\alpha\boldsymbol{k}\sigma}\, |\nu_{\mathrm{L}}, \nu_{\mathrm{R}}\rangle\, \langle m|\, d^{\dagger}_{\mu}\, |n\rangle \\ &\times \langle \nu_{\mathrm{R}}, \nu_{\mathrm{L}}|\, a^{\dagger}_{\alpha\boldsymbol{k}\sigma} a_{\alpha\boldsymbol{k}\sigma}\, |\nu_{\mathrm{L}}, \nu_{\mathrm{R}}\rangle\, \langle n|\, d_{\mu}\, |m\rangle\, \delta\left(E_i - E_f\right) \\ &+ \frac{2\pi}{\hbar}\sum_{\alpha\mu\boldsymbol{k}\sigma}\sum_{\nu_{\mathrm{L}},\nu_{\mathrm{R}}} \left|t_{\alpha\mu\boldsymbol{k}\sigma}\right|^2 W_{\nu_{\mathrm{L}},\nu_{\mathrm{R}}} \langle \nu_{\mathrm{R}}, \nu_{\mathrm{L}}|\, a_{\alpha\boldsymbol{k}\sigma} a^{\dagger}_{\alpha\boldsymbol{k}\sigma}\, |\nu_{\mathrm{L}}, \nu_{\mathrm{R}}\rangle\, \langle m|\, d_{\mu}\, |n\rangle \\ &\times \langle \nu_{\mathrm{R}}, \nu_{\mathrm{L}}|\, a_{\alpha\boldsymbol{k}\sigma} a^{\dagger}_{\alpha\boldsymbol{k}\sigma}\, |\nu_{\mathrm{L}}, \nu_{\mathrm{R}}\rangle\, \langle n|\, d^{\dagger}_{\mu}\, |m\rangle\, \delta\left(E_i - E_f\right), \end{aligned} \tag{2.32}$$

对于费米子, 其粒子数算符 $n_{\alpha\boldsymbol{k}\sigma} = a^{\dagger}_{\alpha\boldsymbol{k}\sigma} a_{\alpha\boldsymbol{k}\sigma}$ 满足 $(n_{\alpha\boldsymbol{k}\sigma})^2 = n_{\alpha\boldsymbol{k}\sigma} = a^{\dagger}_{\alpha\boldsymbol{k}\sigma} a_{\alpha\boldsymbol{k}\sigma}$, 因此, 式 (2.32) 可简化为

$$\begin{aligned} R_{n\to m} =& \frac{2\pi}{\hbar}\sum_{\alpha\mu\boldsymbol{k}\sigma}\sum_{\nu_{\mathrm{L}},\nu_{\mathrm{R}}} \left|t_{\alpha\mu\boldsymbol{k}\sigma}\right|^2 W_{\nu_{\mathrm{L}},\nu_{\mathrm{R}}} \Big[\langle \nu_{\mathrm{R}}, \nu_{\mathrm{L}}|\, a^{\dagger}_{\alpha\boldsymbol{k}\sigma} a_{\alpha\boldsymbol{k}\sigma}\, |\nu_{\mathrm{L}}, \nu_{\mathrm{R}}\rangle \left|\langle n|\, d_{\mu}\, |m\rangle\right|^2 \\ &+ \langle \nu_{\mathrm{R}}, \nu_{\mathrm{L}}|\, a_{\alpha\boldsymbol{k}\sigma} a^{\dagger}_{\alpha\boldsymbol{k}\sigma}\, |\nu_{\mathrm{L}}, \nu_{\mathrm{R}}\rangle \left|\langle m|\, d_{\mu}\, |n\rangle\right|^2\Big]\, \delta\left(E_i - E_f\right), \end{aligned} \tag{2.33}$$

考虑到费米分布函数的性质

$$f\left(\varepsilon_{\alpha\boldsymbol{k}\sigma} - \mu_{\alpha}\right) = \sum_{\nu_{\alpha}} W_{\nu_{\alpha}}\, \langle \nu_{\alpha}|\, a^{\dagger}_{\alpha\boldsymbol{k}\sigma} a_{\alpha\boldsymbol{k}\sigma}\, |\nu_{\alpha}\rangle, \tag{2.34}$$

$$1 - f\left(\varepsilon_{\alpha\boldsymbol{k}\sigma} - \mu_{\alpha}\right) = \sum_{\nu_{\alpha}} W_{\nu_{\alpha}}\, \langle \nu_{\alpha}|\, a_{\alpha\boldsymbol{k}\sigma} a^{\dagger}_{\alpha\boldsymbol{k}\sigma}\, |\nu_{\alpha}\rangle, \tag{2.35}$$

可将式 (2.33) 简化为

$$
\begin{aligned}
R_{n\to m} = & \frac{2\pi}{\hbar}\sum_{\alpha\mu\boldsymbol{k}\sigma}\left|t_{\alpha\mu\boldsymbol{k}\sigma}\right|^2 f\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}-\mu_\alpha\right)\left|\langle n|\, d_\mu\, |m\rangle\right|^2 \delta\left(E_i-E_f\right) \\
& + \frac{2\pi}{\hbar}\sum_{\alpha\mu\boldsymbol{k}\sigma}\left|t_{\alpha\mu\boldsymbol{k}\sigma}\right|^2 \left[1-f\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}-\mu_\alpha\right)\right]\left|\langle m|\, d_\mu\, |n\rangle\right|^2 \delta\left(E_i-E_f\right).
\end{aligned} \tag{2.36}
$$

将式 (2.36) 中对态指标的求和换成积分形式, 并利用式 (2.29) 和式 (2.30), 可将上式写为

$$
\begin{aligned}
R_{n\to m} = & \sum_{\alpha\mu\sigma}\int \mathrm{d}\varepsilon \frac{2\pi}{\hbar}\rho_{\alpha\sigma}\left(\varepsilon\right)\left|t_{\alpha\mu\sigma}\right|^2 f\left(\varepsilon-\mu_\alpha\right)\left|\langle n|\, d_\mu\, |m\rangle\right|^2 \delta\left(\varepsilon_n-\varepsilon_m+\varepsilon\right) \\
& + \sum_{\alpha\mu\sigma}\int \mathrm{d}\varepsilon \frac{2\pi}{\hbar}\rho_{\alpha\sigma}\left(\varepsilon\right)\left|t_{\alpha\mu\sigma}\right|^2 \left[1-f\left(\varepsilon-\mu_\alpha\right)\right]\left|\langle m|\, d_\mu\, |n\rangle\right|^2 \delta\left(\varepsilon_n-\varepsilon_m-\varepsilon\right).
\end{aligned} \tag{2.37}
$$

这里假设隧穿振幅 $t_{\alpha\mu\boldsymbol{k}\sigma}$ 不依赖于波矢量 $\boldsymbol{k}$. 利用 $\delta$ 函数的性质, 可将式 (2.37) 写为 [2,3]

$$
R_{n\to m} = \sum_{\alpha\mu\sigma}\Gamma_{\alpha\mu\sigma}\left\{f\left(\varepsilon_m-\varepsilon_n-\mu_\alpha\right)\left|D^\mu_{nm}\right|^2 + \left[1-f\left(\varepsilon_n-\varepsilon_m-\mu_\alpha\right)\right]\left|D^\mu_{mn}\right|^2\right\}, \tag{2.38}
$$

其中

$$
\Gamma_{\alpha\mu\sigma} = \frac{2\pi\rho_{\alpha\sigma}\left(\varepsilon\right)\left|t_{\alpha\mu\sigma}\right|^2}{\hbar}, \tag{2.39}
$$

$$
D^\mu_{nm} = \langle n|\, d_\mu\, |m\rangle\,. \tag{2.40}
$$

这里, 特别需要指出的是, 对于式 (2.28) 和式 (2.38) 描述的率方程, 仅考虑了所研究量子系统的密度矩阵对角元, 因此, 并不能解决该体系中与其相干性关联的问题.

## 2.3 马尔可夫的量子主方程

为了研究量子相干性对开放量子系统电子输运特性的影响, 下面, 推导可以自洽包含量子系统约化密度矩阵非对角元的马尔可夫量子主方程. 在相互作用绘景中, 由式 (1.33) 可知整个开放量子系统的密度算符演化方程为

$$
\mathrm{i}\hbar\frac{\partial\rho_{\mathrm{I}}\left(t\right)}{\partial t} = \left[H_{\mathrm{T,I}}\left(t\right), \rho_{\mathrm{I}}\left(t\right)\right], \tag{2.41}
$$

对式 (2.41) 两边求关于时间 $t$ 的积分可得

$$
\rho_{\mathrm{I}}\left(t\right) = \rho_{\mathrm{I}}\left(0\right) - \frac{\mathrm{i}}{\hbar}\int_0^t \mathrm{d}t'\left[H_{\mathrm{T,I}}\left(t'\right), \rho_{\mathrm{I}}\left(t'\right)\right], \tag{2.42}
$$

这里取 $t_0 = 0$. 将式 (2.42) 代入式 (2.41) 可得

$$\frac{\partial \rho_{\mathrm{I}}(t)}{\partial t} = -\frac{\mathrm{i}}{\hbar}\left[H_{\mathrm{T,I}}(t), \rho_{\mathrm{I}}(0)\right] - \frac{1}{\hbar^2}\int_0^t \mathrm{d}t' \left[H_{\mathrm{T,I}}(t), \left[H_{\mathrm{T,I}}(t'), \rho_{\mathrm{I}}(t')\right]\right], \tag{2.43}$$

在典型的量子输运问题中, 所研究的量子系统通常对电子库, 即对源极和漏极的电子分布状态影响很小, 并且两者之间的关联可以忽略. 因而, 整个开放量子系统的密度算符 $\rho_{\mathrm{I}}(t)$ 可以写成量子系统的密度算符 $\rho_{\mathrm{QS,I}}(t)$ 和电子库的密度算符 $\rho_{\mathrm{leads}}(t)$ 的直积

$$\rho_{\mathrm{I}}(t) = \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}}(t), \tag{2.44}$$

其中 $\rho_{\mathrm{QS,I}}(t) = \mathrm{tr}_{\mathrm{leads}}\left[\rho_{\mathrm{I}}(t)\right]$. 对式 (2.43) 两边求关于电极的迹, 可得开放量子系统约化密度矩阵的演化方程

$$\frac{\partial \rho_{\mathrm{QS,I}}(t)}{\partial t} = -\frac{1}{\hbar^2}\mathrm{tr}_{\mathrm{leads}}\int_0^t \mathrm{d}t' \left[H_{\mathrm{T,I}}(t), \left[H_{\mathrm{T,I}}(t'), \rho_{\mathrm{I}}(t')\right]\right], \tag{2.45}$$

其中, 对于式 (2.43) 右边第一项关于电极的迹, 由于 $H_{\mathrm{T,I}}(t)$ 是所研究量子系统和电子库算符的线性组合, 见式 (2.4), 因此有

$$-\frac{\mathrm{i}}{\hbar}\mathrm{tr}_{\mathrm{leads}}\left\{\left[H_{\mathrm{T,I}}(t), \rho_{\mathrm{I}}(0)\right]\right\} = 0. \tag{2.46}$$

利用薛定谔绘景和相互作用绘景之间密度算符的变换关系, 即式 (1.31), 可得

$$\begin{aligned}
\frac{\mathrm{d}\rho_{\mathrm{I}}(t)}{\mathrm{d}t} =& \frac{\mathrm{i}}{\hbar}\mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t/\hbar}\left(H_{\mathrm{QS}}+H_{\mathrm{leads}}\right)\rho_{\mathrm{S}}(t)\,\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t/\hbar} \\
&+ \mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t/\hbar}\frac{\mathrm{d}\rho_{\mathrm{S}}(t)}{\mathrm{d}t}\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t/\hbar} \\
&- \frac{\mathrm{i}}{\hbar}\mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t/\hbar}\rho_{\mathrm{S}}(t)\left(H_{\mathrm{QS}}+H_{\mathrm{leads}}\right)\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t/\hbar} \\
=& \mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t/\hbar}\left\{\frac{\mathrm{d}\rho_{\mathrm{S}}(t)}{\mathrm{d}t} + \frac{\mathrm{i}}{\hbar}\left[H_{\mathrm{QS}}+H_{\mathrm{leads}}, \rho_{\mathrm{S}}(t)\right]\right\}\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t/\hbar},
\end{aligned} \tag{2.47}$$

将式 (2.47) 两边分别左乘 $\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t/\hbar}$ 和右乘 $\mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t/\hbar}$, 并对其求关于电极的迹可得

$$\begin{aligned}
&\frac{\mathrm{d}\rho_{\mathrm{QS}}(t)}{\mathrm{d}t} \\
=& -\frac{\mathrm{i}}{\hbar}\left[H_{\mathrm{QS}}, \rho_{\mathrm{QS}}(t)\right] + \mathrm{tr}_{\mathrm{leads}}\left[\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t/\hbar}\frac{\partial \rho_{\mathrm{I}}(t)}{\partial t}\mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t/\hbar}\right],
\end{aligned} \tag{2.48}$$

将式 (2.43) 代入式 (2.48)，可得开放量子系统的约化密度矩阵 $\rho_{\mathrm{QS,I}}(t)$ 在薛定谔绘景中的演化方程

$$
\begin{aligned}
&\frac{\mathrm{d}\rho_{\mathrm{QS}}(t)}{\mathrm{d}t}\\
=&-\frac{\mathrm{i}}{\hbar}\left[H_{\mathrm{QS}},\rho_{\mathrm{QS}}(t)\right]\\
&-\frac{1}{\hbar^2}\mathrm{tr}_{\mathrm{leads}}\left[\int_0^t \mathrm{d}t' H_{\mathrm{T}}\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})\left(t-t'\right)/\hbar}H_{\mathrm{T}}\rho_{\mathrm{QS}}(t')\otimes\rho_{\mathrm{leads}}\mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})\left(t-t'\right)/\hbar}\right]\\
&+\frac{1}{\hbar^2}\mathrm{tr}_{\mathrm{leads}}\left[\int_0^t \mathrm{d}t' H_{\mathrm{T}}\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})\left(t-t'\right)/\hbar}\rho_{\mathrm{QS}}(t')\otimes\rho_{\mathrm{leads}}H_{\mathrm{T}}\mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})\left(t-t'\right)/\hbar}\right]\\
&+\frac{1}{\hbar^2}\mathrm{tr}_{\mathrm{leads}}\left[\int_0^t \mathrm{d}t' \mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})\left(t-t'\right)/\hbar}H_{\mathrm{T}}\rho_{\mathrm{QS}}(t')\otimes\rho_{\mathrm{leads}}\mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})\left(t-t'\right)/\hbar}H_{\mathrm{T}}\right]\\
&-\frac{1}{\hbar^2}\mathrm{tr}_{\mathrm{leads}}\left[\int_0^t \mathrm{d}t' \mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})\left(t-t'\right)/\hbar}\rho_{\mathrm{QS}}(t')\otimes\rho_{\mathrm{leads}}H_{\mathrm{T}}\mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})\left(t-t'\right)/\hbar}H_{\mathrm{T}}\right].
\end{aligned}
\tag{2.49}
$$

由式 (2.49) 可知, 电极的时间关联函数依赖于时间间隔 $t-t'$. 对于通常的电极, 其电子库足够大, 因而可以很快消除由于与所研究的量子系统相互作用而引起的效应. 所以, 仅当此时间间隔 $t-t'$ 小于电极的关联时间 $\tau$, 或者与电极的关联时间 $\tau$ 处于同一量级, 即 $t'$ 在 $t'\approx t-\tau$ 和 $t'=t$ 之间时, 其关联函数的数值才不为零. 尤其是, 当 $t'$ 不在上述时间间隔内时, 密度矩阵 $\rho_{\mathrm{I}}(t')$ 对其在 $t$ 时刻的 $\rho_{\mathrm{I}}(t)$ 影响很小. 仅当此时间间隔 $t-t'$ 不远大于电极的关联时间 $\tau$ 时, 系统才能保持其记忆效应, 即非马尔可夫效应. 这里, 考虑关联时间 $\tau$ 远小于所研究量子系统密度算符 $\rho_{\mathrm{QS}}(t)$ 在宏观上有明显变化的特征时间 $1/T_{\mathrm{QS}}$, 因而式 (2.49) 中的 $\rho_{\mathrm{I}}(t')$ 可以用 $\rho_{\mathrm{I}}(t)$ 替换, 此即所谓的马尔可夫近似 [4,5]. 若令 $t''=t-t'$, 由于当 $t''\gg\tau$, 关联函数等效为零, 此时, 可将式 (2.49) 中的积分上限拓展到无穷, 即

$$
\int_0^t \mathrm{d}t' = \int_t^0 -\mathrm{d}t'' \overset{t=\infty}{=} \int_\infty^0 -\mathrm{d}t'' = \int_0^\infty \mathrm{d}t'', \tag{2.50}
$$

因而, 式 (2.49) 可重新表示为

$$
\frac{\mathrm{d}\rho_{\mathrm{QS}}(t)}{\mathrm{d}t} = -\frac{\mathrm{i}}{\hbar}\left[H_{\mathrm{QS}},\rho_{\mathrm{QS}}(t)\right] + \rho_{\mathrm{QS}}\big|_1 + \rho_{\mathrm{QS}}\big|_2 + \rho_{\mathrm{QS}}\big|_3 + \rho_{\mathrm{QS}}\big|_4, \tag{2.51}
$$

其中

$$
\begin{aligned}
\rho_{\mathrm{QS}}\big|_1 =& -\frac{1}{\hbar^2}\mathrm{tr}_{\mathrm{leads}}\left[\int_0^\infty \mathrm{d}t'' H_{\mathrm{T}}\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t''/\hbar}\right.\\
&\left.\times H_{\mathrm{T}}\mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t''/\hbar}\rho_{\mathrm{QS}}(t)\otimes\rho_{\mathrm{leads}}\right],
\end{aligned}
\tag{2.52}
$$

$$
\rho_{\mathrm{QS}}\big|_2 = \frac{1}{\hbar^2}\mathrm{tr}_{\mathrm{leads}}\left[\int_0^\infty \mathrm{d}t'' H_{\mathrm{T}}\rho_{\mathrm{QS}}(t)\otimes\rho_{\mathrm{leads}}\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t''/\hbar}\right.
$$

$$\times H_{\mathrm{T}}\mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t''/\hbar}\Big], \tag{2.53}$$

$$\begin{aligned}\rho_{\mathrm{QS}}\big|_3 = &\frac{1}{\hbar^2}\mathrm{tr}_{\mathrm{leads}}\Big[\int_0^{\infty}\mathrm{d}t''\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t''/\hbar}\\ &\times H_{\mathrm{T}}\mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t''/\hbar}\rho_{\mathrm{QS}}\left(t\right)\otimes\rho_{\mathrm{leads}}H_{\mathrm{T}}\Big],\end{aligned} \tag{2.54}$$

$$\begin{aligned}\rho_{\mathrm{QS}}\big|_4 = &-\frac{1}{\hbar^2}\mathrm{tr}_{\mathrm{leads}}\Big[\int_0^{\infty}\mathrm{d}t''\rho_{\mathrm{QS}}\left(t\right)\otimes\rho_{\mathrm{leads}}\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t''/\hbar}\\ &\times H_{\mathrm{T}}\mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t''/\hbar}H_{\mathrm{T}}\Big].\end{aligned} \tag{2.55}$$

将式 (2.4) 代入式 (2.52) 可得

$$\begin{aligned}\rho_{\mathrm{QS}}\big|_1 = &-\frac{1}{\hbar^2}\sum_{\alpha\mu\boldsymbol{k}\sigma}\sum_{\alpha'\mu'\boldsymbol{k}'\sigma'}\int_0^{\infty}\mathrm{d}t''t_{\alpha\mu\boldsymbol{k}\sigma}t^*_{\alpha'\mu'\boldsymbol{k}'\sigma'}\mathrm{tr}_{\mathrm{leads}}d^\dagger_\mu a_{\alpha\boldsymbol{k}\sigma}\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t''/\hbar}\\ &\times\mathrm{e}^{-\mathrm{i}H_{\mathrm{leads}}t''/\hbar}a^\dagger_{\alpha'\boldsymbol{k}'\sigma'}\mathrm{e}^{\mathrm{i}H_{\mathrm{leads}}t''/\hbar}d_{\mu'}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t''/\hbar}\rho_{\mathrm{QS}}\left(t\right)\otimes\rho_{\mathrm{leads}}\\ &-\frac{1}{\hbar^2}\sum_{\alpha\mu\boldsymbol{k}\sigma}\sum_{\alpha'\mu'\boldsymbol{k}'\sigma'}\int_0^{\infty}\mathrm{d}t''t^*_{\alpha\mu\boldsymbol{k}\sigma}t_{\alpha'\mu'\boldsymbol{k}'\sigma'}\mathrm{tr}_{\mathrm{leads}}a^\dagger_{\alpha\boldsymbol{k}\sigma}d_\mu\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t''/\hbar}d^\dagger_{\mu'}\\ &\times\mathrm{e}^{-\mathrm{i}H_{\mathrm{leads}}t''/\hbar}a_{\alpha'\boldsymbol{k}'\sigma'}\mathrm{e}^{\mathrm{i}H_{\mathrm{leads}}t''/\hbar}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t''/\hbar}\rho_{\mathrm{QS}}\left(t\right)\otimes\rho_{\mathrm{leads}},\end{aligned} \tag{2.56}$$

利用如下的关系式:

$$\mathrm{e}^{-\mathrm{i}H_{\mathrm{leads}}t''/\hbar}a^\dagger_{\alpha'\boldsymbol{k}'\sigma'}\mathrm{e}^{\mathrm{i}H_{\mathrm{leads}}t''/\hbar}=\mathrm{e}^{-\mathrm{i}\varepsilon_{\alpha'\boldsymbol{k}'\sigma'}t''/\hbar}a^\dagger_{\alpha'\boldsymbol{k}'\sigma'}, \tag{2.57}$$

$$\mathrm{e}^{-\mathrm{i}H_{\mathrm{leads}}t''/\hbar}a_{\alpha'\boldsymbol{k}'\sigma'}\mathrm{e}^{\mathrm{i}H_{\mathrm{leads}}t''/\hbar}=\mathrm{e}^{\mathrm{i}\varepsilon_{\alpha'\boldsymbol{k}'\sigma'}t''/\hbar}a_{\alpha'\boldsymbol{k}'\sigma'}, \tag{2.58}$$

可将式 (2.56) 写为

$$\begin{aligned}&\rho_{\mathrm{QS}}\big|_1\\ = &-\frac{1}{\hbar^2}\sum_{\alpha\mu\boldsymbol{k}\sigma}\sum_{\alpha'\mu'\boldsymbol{k}'\sigma'}t_{\alpha\mu\boldsymbol{k}\sigma}t^*_{\alpha'\mu'\boldsymbol{k}'\sigma'}\int_0^{\infty}\mathrm{d}t''\mathrm{e}^{-i\varepsilon_{\alpha'\boldsymbol{k}'\sigma'}t''/\hbar}\mathrm{tr}_{\mathrm{leads}}\left(a_{\alpha\boldsymbol{k}\sigma}a^\dagger_{\alpha'\boldsymbol{k}'\sigma'}\rho_{\mathrm{leads}}\right)d^\dagger_\mu\\ &\times\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t''/\hbar}d_{\mu'}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t''/\hbar}\rho_{\mathrm{QS}}\left(t\right)\\ &-\frac{1}{\hbar^2}\sum_{\alpha\mu\boldsymbol{k}\sigma}\sum_{\alpha'\mu'\boldsymbol{k}'\sigma'}t^*_{\alpha\mu\boldsymbol{k}\sigma}t_{\alpha'\mu'\boldsymbol{k}'\sigma'}\int_0^{\infty}\mathrm{d}t''\mathrm{e}^{\mathrm{i}\varepsilon_{\alpha'\boldsymbol{k}'\sigma'}t''/\hbar}\mathrm{tr}_{\mathrm{leads}}\left(a^\dagger_{\alpha\boldsymbol{k}\sigma}a_{\alpha'\boldsymbol{k}'\sigma'}\rho_{\mathrm{leads}}\right)d_\mu\\ &\times\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t''/\hbar}d^\dagger_{\mu'}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t''/\hbar}\rho_{\mathrm{QS}}\left(t\right).\end{aligned} \tag{2.59}$$

另外, 由式 (2.34) 和式 (2.35) 可知,

$$\mathrm{tr}_{\mathrm{leads}}\left(a^\dagger_{\alpha\boldsymbol{k}\sigma}a_{\alpha'\boldsymbol{k}'\sigma'}\rho_{\mathrm{leads}}\right)=\delta_{\alpha\alpha'}\delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\sigma\sigma'}f\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}-\mu_\alpha\right)=f^{(+)}_\alpha\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\right), \tag{2.60}$$

$$\mathrm{tr}_{\mathrm{leads}}\left(a_{\alpha\boldsymbol{k}\sigma}a^{\dagger}_{\alpha'\boldsymbol{k}'\sigma'}\rho_{\mathrm{leads}}\right)=\delta_{\alpha\alpha'}\delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\sigma\sigma'}\left[1-f\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}-\mu_{\alpha}\right)\right]=f^{(-)}_{\alpha}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\right),\tag{2.61}$$

因而, 式 (2.59) 可以表示为

$$\begin{aligned}&\rho_{\mathrm{QS}}|_1\\&=-\sum_{\alpha\boldsymbol{k}\sigma}\sum_{\mu\mu'}\frac{|t_{\alpha\boldsymbol{k}\sigma}|^2_{\mu\mu'}}{\hbar^2}\int_0^{\infty}\mathrm{d}t''\mathrm{e}^{-\mathrm{i}\varepsilon_{\alpha\boldsymbol{k}\sigma}t''/\hbar}f^{(-)}_{\alpha}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\right)d^{\dagger}_{\mu}\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t''/\hbar}d_{\mu'}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t''/\hbar}\rho_{\mathrm{QS}}\left(t\right)\\&\quad-\sum_{\alpha\boldsymbol{k}\sigma}\sum_{\mu\mu'}\frac{|t_{\alpha\boldsymbol{k}\sigma}|^2_{\mu\mu'}}{\hbar^2}\int_0^{\infty}\mathrm{d}t''\mathrm{e}^{\mathrm{i}\varepsilon_{\alpha\boldsymbol{k}\sigma}t''/\hbar}f^{(+)}_{\alpha}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\right)d_{\mu}\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t''/\hbar}d^{\dagger}_{\mu'}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t''/\hbar}\rho_{\mathrm{QS}}\left(t\right).\end{aligned}\tag{2.62}$$

由算符函数的性质 [6]

$$\mathrm{e}^{A}B\mathrm{e}^{-A}=B+\frac{1}{1!}\left[A,B\right]+\frac{1}{2!}\left[A,\left[A,B\right]\right]+\frac{1}{3!}\left[A,\left[A,\left[A,B\right]\right]\right]+\cdots=\mathrm{e}^{L}B,\tag{2.63}$$

其中, 算符 $L$ 定义为 $L=[A,B]$. 根据式 (2.63) 的定义, 式 (2.62) 可进一步简化为

$$\begin{aligned}\rho_{\mathrm{QS}}|_1=&-\sum_{\alpha\boldsymbol{k}\sigma}\sum_{\mu\mu'}\frac{|t_{\alpha\boldsymbol{k}\sigma}|^2_{\mu\mu'}}{\hbar^2}\int_0^{\infty}\mathrm{d}t''f^{(-)}_{\alpha}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\right)d^{\dagger}_{\mu}\left[\mathrm{e}^{-\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}+L_{\mathrm{QS}})t''/\hbar}d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)\\&-\sum_{\alpha\boldsymbol{k}\sigma}\sum_{\mu\mu'}\frac{|t_{\alpha\boldsymbol{k}\sigma}|^2_{\mu\mu'}}{\hbar^2}\int_0^{\infty}\mathrm{d}t''f^{(+)}_{\alpha}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\right)d_{\mu}\left[\mathrm{e}^{\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}-L_{\mathrm{QS}})t''/\hbar}d^{\dagger}_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right),\end{aligned}\tag{2.64}$$

其中, $L_{\mathrm{QS}}d_{\mu}\left(d^{\dagger}_{\mu}\right)=\left[H_{\mathrm{QS}},d_{\mu}\left(d^{\dagger}_{\mu}\right)\right]$.

同理, 可以将式 (2.53) ~ 式 (2.55) 简化为

$$\begin{aligned}\rho_{\mathrm{QS}}|_2=&\sum_{\alpha\boldsymbol{k}\sigma}\sum_{\mu\mu'}\frac{|t_{\alpha\boldsymbol{k}\sigma}|^2_{\mu\mu'}}{\hbar^2}\int_0^{\infty}\mathrm{d}t''f^{(+)}_{\alpha}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\right)d^{\dagger}_{\mu}\rho_{\mathrm{QS}}\left(t\right)\left[\mathrm{e}^{-\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}+L_{\mathrm{QS}})t''/\hbar}d_{\mu'}\right]\\&+\sum_{\alpha\boldsymbol{k}\sigma}\sum_{\mu\mu'}\frac{|t_{\alpha\boldsymbol{k}\sigma}|^2_{\mu\mu'}}{\hbar^2}\int_0^{\infty}\mathrm{d}t''f^{(-)}_{\alpha}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\right)d_{\mu}\rho_{\mathrm{QS}}\left(t\right)\left[\mathrm{e}^{\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}-L_{\mathrm{QS}})t''/\hbar}d^{\dagger}_{\mu'}\right],\end{aligned}\tag{2.65}$$

$$\begin{aligned}\rho_{\mathrm{QS}}|_3=&\sum_{\alpha\boldsymbol{k}\sigma}\sum_{\mu\mu'}\frac{|t_{\alpha\boldsymbol{k}\sigma}|^2_{\mu\mu'}}{\hbar^2}\int_0^{\infty}\mathrm{d}t''f^{(+)}_{\alpha}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\right)\left[\mathrm{e}^{\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}-L_{\mathrm{QS}})t''/\hbar}d^{\dagger}_{\mu}\right]\rho_{\mathrm{QS}}\left(t\right)d_{\mu'}\\&+\sum_{\alpha\boldsymbol{k}\sigma}\sum_{\mu\mu'}\frac{|t_{\alpha\boldsymbol{k}\sigma}|^2_{\mu\mu'}}{\hbar^2}\int_0^{\infty}\mathrm{d}t''f^{(-)}_{\alpha}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\right)\left[\mathrm{e}^{-\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}+L_{\mathrm{QS}})t''/\hbar}d_{\mu}\right]\rho_{\mathrm{QS}}\left(t\right)d^{\dagger}_{\mu'},\end{aligned}\tag{2.66}$$

$$\rho_{\mathrm{QS}}|_4=-\sum_{\alpha\boldsymbol{k}\sigma}\sum_{\mu\mu'}\frac{|t_{\alpha\boldsymbol{k}\sigma}|^2_{\mu\mu'}}{\hbar^2}\int_0^{\infty}\mathrm{d}t''f^{(-)}_{\alpha}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\right)\rho_{\mathrm{QS}}\left(t\right)\left[\mathrm{e}^{\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}-L_{\mathrm{QS}})t''/\hbar}d^{\dagger}_{\mu}\right]d_{\mu'}$$

$$
-\sum_{\alpha\boldsymbol{k}\sigma}\sum_{\mu\mu'}\frac{\left|t_{\alpha\boldsymbol{k}\sigma}\right|^2_{\mu\mu'}}{\hbar^2}\int_0^{\infty}\mathrm{d}t'' f_{\alpha}^{(+)}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\right)\rho_{\mathrm{QS}}\left(t\right)\left[\mathrm{e}^{-\mathrm{i}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}+L_{\mathrm{QS}}\right)t''/\hbar}d_{\mu}\right]d_{\mu'}^{\dagger}. \tag{2.67}
$$

因而, 在马尔可夫近似下, 若所研究的量子系统与电极的隧穿耦合不依赖于波矢 $\boldsymbol{k}$, 即 $t_{\alpha\mu\boldsymbol{k}\sigma}\equiv t_{\alpha\mu\sigma}$, 则式 (2.51) 可进一步简化为

$$
\frac{\mathrm{d}\rho_{\mathrm{QS}}\left(t\right)}{\mathrm{d}t}=-\frac{\mathrm{i}}{\hbar}\left[H_{\mathrm{QS}},\rho_{\mathrm{QS}}\left(t\right)\right]+\left(A+B+C+D\right), \tag{2.68}
$$

其中

$$
\begin{aligned}
A=&-\sum_{\alpha\sigma,\mu\mu'}\frac{\left|t_{\alpha\sigma}\right|^2_{\mu\mu'}}{\hbar^2}d_{\mu}^{\dagger}\left[\int\mathrm{d}\varepsilon\rho_{\alpha\sigma}\left(\varepsilon\right)f_{\alpha}^{(-)}\left(\varepsilon\right)\int_0^{\infty}\mathrm{d}t''\mathrm{e}^{-\mathrm{i}\left(\varepsilon+L_{\mathrm{QS}}\right)t''/\hbar}d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)\\
&-\sum_{\alpha\sigma,\mu\mu'}\frac{\left|t_{\alpha\sigma}\right|^2_{\mu\mu'}}{\hbar^2}\rho_{\mathrm{QS}}\left(t\right)\left[\int\mathrm{d}\varepsilon\rho_{\alpha\sigma}\left(\varepsilon\right)f_{\alpha}^{(-)}\left(\varepsilon\right)\int_0^{\infty}\mathrm{d}t''\mathrm{e}^{\mathrm{i}\left(\varepsilon-L_{\mathrm{QS}}\right)t''/\hbar}d_{\mu'}^{\dagger}\right]d_{\mu},
\end{aligned} \tag{2.69}
$$

$$
\begin{aligned}
B=&-\sum_{\alpha\sigma,\mu\mu'}\frac{\left|t_{\alpha\sigma}\right|^2_{\mu\mu'}}{\hbar^2}\rho_{\mathrm{QS}}\left(t\right)\left[\int\mathrm{d}\varepsilon\rho_{\alpha\sigma}\left(\varepsilon\right)f_{\alpha}^{(+)}\left(\varepsilon\right)\int_0^{\infty}\mathrm{d}t''\mathrm{e}^{-\mathrm{i}\left(\varepsilon+L_{\mathrm{QS}}\right)t''/\hbar}d_{\mu'}\right]d_{\mu}^{\dagger}\\
&-\sum_{\alpha\sigma,\mu\mu'}\frac{\left|t_{\alpha\sigma}\right|^2_{\mu\mu'}}{\hbar^2}d_{\mu}\left[\int\mathrm{d}\varepsilon\rho_{\alpha\sigma}\left(\varepsilon\right)f_{\alpha}^{(+)}\left(\varepsilon\right)\int_0^{\infty}\mathrm{d}t''\mathrm{e}^{\mathrm{i}\left(\varepsilon-L_{\mathrm{QS}}\right)t''/\hbar}d_{\mu'}^{\dagger}\right]\rho_{\mathrm{QS}}\left(t\right),
\end{aligned} \tag{2.70}
$$

$$
\begin{aligned}
C=&\sum_{\alpha\sigma,\mu\mu'}\frac{\left|t_{\alpha\sigma}\right|^2_{\mu\mu'}}{\hbar^2}d_{\mu}^{\dagger}\rho_{\mathrm{QS}}\left(t\right)\left[\int\mathrm{d}\varepsilon\rho_{\alpha\sigma}\left(\varepsilon\right)f_{\alpha}^{(+)}\left(\varepsilon\right)\int_0^{\infty}\mathrm{d}t''\mathrm{e}^{-\mathrm{i}\left(\varepsilon+L_{\mathrm{QS}}\right)t''/\hbar}d_{\mu'}\right]\\
&+\sum_{\alpha\sigma,\mu\mu'}\frac{\left|t_{\alpha\sigma}\right|^2_{\mu\mu'}}{\hbar^2}\left[\int\mathrm{d}\varepsilon\rho_{\alpha\sigma}\left(\varepsilon\right)f_{\alpha}^{(+)}\left(\varepsilon\right)\int_0^{\infty}\mathrm{d}t''\mathrm{e}^{\mathrm{i}\left(\varepsilon-L_{\mathrm{QS}}\right)t''/\hbar}d_{\mu'}^{\dagger}\right]\rho_{\mathrm{QS}}\left(t\right)d_{\mu},
\end{aligned} \tag{2.71}
$$

$$
\begin{aligned}
D=&\sum_{\alpha\sigma,\mu\mu'}\frac{\left|t_{\alpha\sigma}\right|^2_{\mu\mu'}}{\hbar^2}\left[\int\mathrm{d}\varepsilon\rho_{\alpha\sigma}\left(\varepsilon\right)f_{\alpha}^{(-)}\left(\varepsilon\right)\int_0^{\infty}\mathrm{d}t''\mathrm{e}^{-\mathrm{i}\left(\varepsilon+L_{\mathrm{QS}}\right)t''/\hbar}d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)d_{\mu}^{\dagger}\\
&+\sum_{\alpha\sigma,\mu\mu'}\frac{\left|t_{\alpha\sigma}\right|^2_{\mu\mu'}}{\hbar^2}d_{\mu}\rho_{\mathrm{QS}}\left(t\right)\left[\int\mathrm{d}\varepsilon\rho_{\alpha\sigma}\left(\varepsilon\right)f_{\alpha}^{(-)}\left(\varepsilon\right)\int_0^{\infty}\mathrm{d}t''\mathrm{e}^{\mathrm{i}\left(\varepsilon-L_{\mathrm{QS}}\right)t''/\hbar}d_{\mu'}^{\dagger}\right].
\end{aligned} \tag{2.72}
$$

在马尔可夫近似下, 当时间 $t\to\infty$ 时, 其关联函数的数值将为零, 因而式 (2.69) ~ 式 (2.72) 中的积分

$$
\int_0^{\infty}\mathrm{d}t''\mathrm{e}^{-\mathrm{i}\left(\varepsilon+L_{\mathrm{QS}}\right)t''/\hbar}, \tag{2.73}
$$

可以写为

$$
\begin{aligned}
\int_0^\infty \mathrm{d}t''\mathrm{e}^{-\mathrm{i}(\varepsilon+L_{\mathrm{QS}})t''/\hbar} &= \lim_{\eta\to 0^+}\int_0^\infty \mathrm{d}t''\mathrm{e}^{-\mathrm{i}(\varepsilon+L_{\mathrm{QS}})t''/\hbar}\mathrm{e}^{-\eta t''} = \lim_{\eta\to 0^+}\frac{-\mathrm{i}\hbar}{\varepsilon+L_{\mathrm{QS}}-\mathrm{i}\eta\hbar}\\
&= -\lim_{\eta\to 0^+}\frac{\mathrm{i}\hbar\left(\varepsilon+L_{\mathrm{QS}}\right)}{\left(\varepsilon+L_{\mathrm{QS}}\right)^2+\left(\eta\hbar\right)^2}+\lim_{\eta\hbar\to 0^+}\frac{\hbar\left(\eta\hbar\right)}{\left(\varepsilon+L_{\mathrm{QS}}\right)^2+\left(\eta\hbar\right)^2}\\
&= -\mathrm{i}\hbar P\frac{1}{\varepsilon+L_{\mathrm{QS}}}+\hbar\pi\delta\left(\varepsilon+L_{\mathrm{QS}}\right),
\end{aligned}\tag{2.74}
$$

其中 $P$ 表示积分主值. 同理, 式 (2.69) ~ 式 (2.72) 中的积分 $\int_0^\infty \mathrm{d}t''\mathrm{e}^{\mathrm{i}(\varepsilon-L_{\mathrm{QS}})t''/\hbar}$ 可以写为

$$
\begin{aligned}
&\int_0^\infty \mathrm{d}t''\mathrm{e}^{\mathrm{i}(\varepsilon-L_{\mathrm{QS}})t''/\hbar}\\
&= \lim_{\eta\to 0^+}\int_0^\infty \mathrm{d}t''\mathrm{e}^{\mathrm{i}(\varepsilon-L_{\mathrm{QS}})t''/\hbar}\mathrm{e}^{-\eta t''} = \lim_{\eta\to 0^+}\frac{\mathrm{i}\hbar}{\varepsilon-L_{\mathrm{QS}}+\mathrm{i}\eta\hbar}\\
&= \lim_{\eta\to 0^+}\frac{\mathrm{i}\hbar\left(\varepsilon-L_{\mathrm{QS}}\right)}{\left(\varepsilon-L_{\mathrm{QS}}\right)^2+\left(\eta\hbar\right)^2}+\lim_{\eta\hbar\to 0^+}\frac{\hbar\left(\eta\hbar\right)}{\left(\varepsilon-L_{\mathrm{QS}}\right)^2+\left(\eta\hbar\right)^2}\\
&= \mathrm{i}\hbar P\frac{1}{\varepsilon-L_{\mathrm{QS}}}+\hbar\pi\delta\left(\varepsilon-L_{\mathrm{QS}}\right),
\end{aligned}\tag{2.75}
$$

利用式 (2.74) 和 (2.75), 可将式 (2.69) ~ 式 (2.72) 写为

$$
\begin{aligned}
A = &-\sum_{\alpha\sigma,\mu\mu'}\frac{\pi\left|t_{\alpha\sigma}\right|_{\mu\mu'}}{\hbar}d_\mu^\dagger\left[\int \mathrm{d}\varepsilon\rho_{\alpha\sigma}\left(\varepsilon\right)f_\alpha^{(-)}\left(\varepsilon\right)\delta\left(\varepsilon+L_{\mathrm{QS}}\right)d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)\\
&-\sum_{\alpha\sigma,\mu\mu'}\frac{\pi\left|t_{\alpha\sigma}\right|^2_{\mu\mu'}}{\hbar}\rho_{\mathrm{QS}}\left(t\right)\left[\int \mathrm{d}\varepsilon\rho_{\alpha\sigma}\left(\varepsilon\right)f_\alpha^{(-)}\left(\varepsilon\right)\delta\left(\varepsilon-L_{\mathrm{QS}}\right)d_{\mu'}^\dagger\right]d_\mu\\
&+\mathrm{i}\sum_{\alpha\sigma,\mu\mu'}\frac{\left|t_{\alpha\sigma}\right|^2_{\mu\mu'}}{\hbar}\left\{d_\mu^\dagger\left[D_\alpha^{(-)}\left(L_{\mathrm{QS}}\right)d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)-\rho_{\mathrm{QS}}\left(t\right)\left[D_\alpha^{(-)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}^\dagger\right]d_\mu\right\},
\end{aligned}\tag{2.76}
$$

$$
\begin{aligned}
B = &-\sum_{\alpha\sigma,\mu\mu'}\frac{\pi\left|t_{\alpha\sigma}\right|^2_{\mu\mu'}}{\hbar}\rho_{\mathrm{QS}}\left(t\right)\left[\int \mathrm{d}\varepsilon\rho_{\alpha\sigma}\left(\varepsilon\right)f_\alpha^{(+)}\left(\varepsilon\right)\delta\left(\varepsilon+L_{\mathrm{QS}}\right)d_{\mu'}\right]d_\mu^\dagger\\
&-\sum_{\alpha\sigma,\mu\mu'}\frac{\pi\left|t_{\alpha\sigma}\right|^2_{\mu\mu'}}{\hbar}d_\mu\left[\int \mathrm{d}\varepsilon\rho_{\alpha\sigma}\left(\varepsilon\right)f_\alpha^{(+)}\left(\varepsilon\right)\delta\left(\varepsilon-L_{\mathrm{QS}}\right)d_{\mu'}^\dagger\right]\rho_{\mathrm{QS}}\left(t\right)\\
&+\mathrm{i}\sum_{\alpha\sigma,\mu\mu'}\frac{\left|t_{\alpha\sigma}\right|^2_{\mu\mu'}}{\hbar}\left\{\rho_{\mathrm{QS}}\left(t\right)\left[D_\alpha^{(+)}\left(L_{\mathrm{QS}}\right)d_{\mu'}\right]d_\mu^\dagger-d_\mu\left[D_\alpha^{(+)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}^\dagger\right]\rho_{\mathrm{QS}}\left(t\right)\right\},
\end{aligned}\tag{2.77}
$$

$$
\begin{aligned}
C=&\sum_{\alpha\sigma,\mu\mu'}\frac{\pi\left|t_{\alpha\sigma}\right|_{\mu\mu'}^{2}}{\hbar}d_{\mu}^{\dagger}\rho_{\mathrm{QS}}\left(t\right)\left[\int\mathrm{d}\varepsilon\rho_{\alpha\sigma}\left(\varepsilon\right)f_{\alpha}^{(+)}\left(\varepsilon\right)\delta\left(\varepsilon+L_{\mathrm{QS}}\right)d_{\mu'}\right]\\
&+\sum_{\alpha\sigma,\mu\mu'}\frac{\pi\left|t_{\alpha\sigma}\right|_{\mu\mu'}^{2}}{\hbar}\left[\int\mathrm{d}\varepsilon\rho_{\alpha\sigma}\left(\varepsilon\right)f_{\alpha}^{(+)}\left(\varepsilon\right)\delta\left(\varepsilon-L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]\rho_{\mathrm{QS}}\left(t\right)d_{\mu}\\
&-\mathrm{i}\sum_{\alpha\sigma,\mu\mu'}\frac{\left|t_{\alpha\sigma}\right|_{\mu\mu'}^{2}}{\hbar}\left\{d_{\mu}^{\dagger}\rho_{\mathrm{QS}}\left(t\right)\left[D_{\alpha}^{(+)}\left(L_{\mathrm{QS}}\right)d_{\mu'}\right]-\left[D_{\alpha}^{(+)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]\rho_{\mathrm{QS}}\left(t\right)d_{\mu}\right\},
\end{aligned}
\tag{2.78}
$$

$$
\begin{aligned}
D=&\sum_{\alpha\sigma,\mu\mu'}\frac{\pi\left|t_{\alpha\sigma}\right|_{\mu\mu'}^{2}}{\hbar}\left[\int\mathrm{d}\varepsilon\rho_{\alpha\sigma}\left(\varepsilon\right)f_{\alpha}^{(-)}\left(\varepsilon\right)\delta\left(\varepsilon+L_{\mathrm{QS}}\right)d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)d_{\mu}^{\dagger}\\
&+\sum_{\alpha\sigma,\mu\mu'}\frac{\pi\left|t_{\alpha\sigma}\right|_{\mu\mu'}^{2}}{\hbar}d_{\mu}\rho_{\mathrm{QS}}\left(t\right)\left[\int\mathrm{d}\varepsilon\rho_{\alpha\sigma}\left(\varepsilon\right)f_{\alpha}^{(-)}\left(\varepsilon\right)\delta\left(\varepsilon-L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]\\
&-\mathrm{i}\sum_{\alpha\sigma,\mu\mu'}\frac{\left|t_{\alpha\sigma}\right|_{\mu\mu'}^{2}}{\hbar}\left\{\left[D_{\alpha}^{(-)}\left(L_{\mathrm{QS}}\right)d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)d_{\mu}^{\dagger}-d_{\mu}\rho_{\mathrm{QS}}\left(t\right)\left[D_{\alpha}^{(-)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]\right\},
\end{aligned}
\tag{2.79}
$$

其中,

$$
D_{\alpha}^{(\pm)}\left(L_{\mathrm{QS}}\right)=P\int\mathrm{d}\varepsilon\frac{\rho_{\alpha\sigma}\left(\varepsilon\right)f_{\alpha}^{(\pm)}\left(\varepsilon\right)}{\varepsilon+L_{\mathrm{QS}}},\tag{2.80}
$$

$$
D_{\alpha}^{(\pm)}\left(-L_{\mathrm{QS}}\right)=P\int\mathrm{d}\varepsilon\frac{\rho_{\alpha\sigma}\left(\varepsilon\right)f_{\alpha}^{(\pm)}\left(\varepsilon\right)}{\varepsilon-L_{\mathrm{QS}}}.\tag{2.81}
$$

若电极的态密度 $\rho_{\alpha\sigma}\left(\varepsilon\right)$ 选择洛伦兹截断 [5], 即

$$
\rho_{\alpha\sigma}\left(\varepsilon\right)=\rho_{\alpha\sigma}\frac{W^{2}}{\left(\varepsilon-\mu_{\alpha}\right)^{2}+W^{2}}=\rho_{\alpha\sigma}g_{\alpha}\left(\varepsilon\right),\tag{2.82}
$$

其中 $\rho_{\alpha\sigma}$ 为常数. 在宽带近似下, 即 $W\gg\varepsilon,\mu_{\alpha},k_{\mathrm{B}}T,\Delta$(在 $H_{\mathrm{QS}}$ 的能量本征态基矢中, 算符 $L_{\mathrm{QS}}$ 刻画了其能级差 $\Delta$), 利用留数定理 [7], 式 (2.80) 和式 (2.81) 中的四个积分主值分别为

$$
D_{\alpha}^{(+)}\left(L_{\mathrm{QS}}\right)=P\int\mathrm{d}\varepsilon\frac{g_{\alpha}\left(\omega\right)f_{\alpha}^{(+)}\left(\varepsilon\right)}{\varepsilon+L_{\mathrm{QS}}}=\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{-L_{\mathrm{QS}}-\mu_{\alpha}}{2\pi k_{\mathrm{B}}T}\right)-\ln\frac{W}{2\pi k_{\mathrm{B}}T},\tag{2.83}
$$

$$
D_{\alpha}^{(-)}\left(L_{\mathrm{QS}}\right)=P\int\mathrm{d}\varepsilon\frac{g_{\alpha}\left(\omega\right)f_{\alpha}^{(-)}\left(\varepsilon\right)}{\varepsilon+L_{\mathrm{QS}}}=-\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{-L_{\mathrm{QS}}-\mu_{\alpha}}{2\pi k_{\mathrm{B}}T}\right)+\ln\frac{W}{2\pi k_{\mathrm{B}}T},\tag{2.84}
$$

$$
D_{\alpha}^{(+)}\left(-L_{\mathrm{QS}}\right)=P\int\mathrm{d}\varepsilon\frac{g_{\alpha}\left(\omega\right)f_{\alpha}^{(+)}\left(\varepsilon\right)}{\varepsilon-L_{\mathrm{QS}}}=\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{L_{\mathrm{QS}}-\mu_{\alpha}}{2\pi k_{\mathrm{B}}T}\right)-\ln\frac{W}{2\pi k_{\mathrm{B}}T},\tag{2.85}
$$

$$D_{\alpha}^{(-)}\left(-L_{\mathrm{QS}}\right)=P\int \mathrm{d}\varepsilon\frac{g_{\alpha}\left(\omega\right)f_{\alpha}^{(-)}\left(\varepsilon\right)}{\varepsilon-L_{\mathrm{QS}}}=-\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{L_{\mathrm{QS}}-\mu_{\alpha}}{2\pi k_{\mathrm{B}}T}\right)+\ln\frac{W}{2\pi k_{\mathrm{B}}T}. \tag{2.86}$$

具体计算过程见附录 A. 若定义 $\Gamma_{\alpha\sigma}^{\mu\mu'}=2\pi\rho_{\alpha\sigma}\left|t_{\alpha\sigma}\right|_{\mu\mu'}^{2}\Big/\hbar$, 则式 (2.76) ~ 式 (2.79) 可进一步简化为

$$\begin{aligned}A=&-\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2}\left\{d_{\mu}^{\dagger}\left[f_{\alpha}^{(-)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)+\rho_{\mathrm{QS}}\left(t\right)\left[f_{\alpha}^{(-)}\left(L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]d_{\mu}\right\}\\&+\mathrm{i}\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2\pi}\left\{d_{\mu}^{\dagger}\left[D_{\alpha}^{(-)}\left(L_{\mathrm{QS}}\right)d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)-\rho_{\mathrm{QS}}\left(t\right)\left[D_{\alpha}^{(-)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]d_{\mu}\right\},\end{aligned} \tag{2.87}$$

$$\begin{aligned}B=&-\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2}\left\{\rho_{\mathrm{QS}}\left(t\right)\left[f_{\alpha}^{(+)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}\right]d_{\mu}^{\dagger}+d_{\mu}\left[f_{\alpha}^{(+)}\left(L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]\rho_{\mathrm{QS}}\left(t\right)\right\}\\&+\mathrm{i}\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2\pi}\left\{\rho_{\mathrm{QS}}\left(t\right)\left[D_{\alpha}^{(+)}\left(L_{\mathrm{QS}}\right)d_{\mu'}\right]d_{\mu}^{\dagger}-d_{\mu}\left[D_{\alpha}^{(+)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]\rho_{\mathrm{QS}}\left(t\right)\right\},\end{aligned} \tag{2.88}$$

$$\begin{aligned}C=&\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2}\left\{d_{\mu}^{\dagger}\rho_{\mathrm{QS}}\left(t\right)\left[f_{\alpha}^{(+)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}\right]+\left[f_{\alpha}^{(+)}\left(L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]\rho_{\mathrm{QS}}\left(t\right)d_{\mu}\right\}\\&-\mathrm{i}\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2\pi}\left\{d_{\mu}^{\dagger}\rho_{\mathrm{QS}}\left(t\right)\left[D_{\alpha}^{(+)}\left(L_{\mathrm{QS}}\right)d_{\mu'}\right]-\left[D_{\alpha}^{(+)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]\rho_{\mathrm{QS}}\left(t\right)d_{\mu}\right\},\end{aligned} \tag{2.89}$$

$$\begin{aligned}D=&\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2}\left\{\left[f_{\alpha}^{(-)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)d_{\mu}^{\dagger}+d_{\mu}\rho_{\mathrm{QS}}\left(t\right)\left[f_{\alpha}^{(-)}\left(L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]\right\}\\&-\mathrm{i}\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2\pi}\left\{\left[D_{\alpha}^{(-)}\left(L_{\mathrm{QS}}\right)d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)d_{\mu}^{\dagger}-d_{\mu}\rho_{\mathrm{QS}}\left(t\right)\left[D_{\alpha}^{(-)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]\right\}.\end{aligned} \tag{2.90}$$

式 (2.87) ~ 式 (2.90) 以及式 (2.68), 即为在马尔可夫近似下, 量子主方程的一般形式. 对于所研究量子系统约化密度矩阵的矩阵元 $\langle m|\,\rho_{\mathrm{QS}}\,|n\rangle$, 这里给出其中一项, 即式 (2.87) 的计算过程. 将式 (2.87) 分别左乘 $\langle m|$ 和右乘 $|n\rangle$ 可得

$$\begin{aligned}\langle m|\,A\,|n\rangle=&-\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2}\langle m|\,d_{\mu}^{\dagger}\left[f_{\alpha}^{(-)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)|n\rangle\\&-\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2}\langle m|\,\rho_{\mathrm{QS}}\left(t\right)\left[f_{\alpha}^{(-)}\left(L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]d_{\mu}\,|n\rangle\end{aligned}$$

$$+\sum_{\alpha\sigma,\mu\mu'}\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{\mu\mu'}}{2\pi}\langle m|\,d_\mu^\dagger\left[D_\alpha^{(-)}\left(L_{\mathrm{QS}}\right)d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)|n\rangle$$
$$-\sum_{\alpha\sigma,\mu\mu'}\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{\mu\mu'}}{2\pi}\langle m|\,\rho_{\mathrm{QS}}\left(t\right)\left[D_\alpha^{(-)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}^\dagger\right]d_\mu\,|n\rangle, \tag{2.91}$$

其中态矢量 $|n\rangle$ 和 $|m\rangle$ 均为哈密顿量 $H_{\mathrm{QS}}$ 的本征态, 见式 (2.27). 若定义 $\langle m|\,d_\mu^\dagger=\langle m'|$, $d_\mu\,|n\rangle=|n'\rangle$, 则式 (2.91) 可以简化为

$$\langle m|\,A\,|n\rangle=-\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2}\langle m'|\left[f_\alpha^{(-)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)|n\rangle$$
$$-\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2}\langle m|\,\rho_{\mathrm{QS}}\left(t\right)\left[f_\alpha^{(-)}\left(L_{\mathrm{QS}}\right)d_{\mu'}^\dagger\right]|n'\rangle$$
$$+\sum_{\alpha\sigma,\mu\mu'}\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{\mu\mu'}}{2\pi}\langle m'|\left[D_\alpha^{(-)}\left(L_{\mathrm{QS}}\right)d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)|n\rangle$$
$$-\sum_{\alpha\sigma,\mu\mu'}\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{\mu\mu'}}{2\pi}\langle m|\,\rho_{\mathrm{QS}}\left(t\right)\left[D_\alpha^{(-)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}^\dagger\right]|n'\rangle\,, \tag{2.92}$$

利用附录 B 中的式 (B.12) 和式 (B.24), 可得

$$\langle m|\,A\,|n\rangle=-\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2}f_\alpha^{(-)}\left(\varepsilon_{m''}-\varepsilon_{m'}\right)\langle m''|\,\rho_{\mathrm{QS}}\left(t\right)|n\rangle$$
$$-\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2}f_\alpha^{(-)}\left(\varepsilon_{n''}-\varepsilon_{n'}\right)\langle m|\,\rho_{\mathrm{QS}}\left(t\right)|n''\rangle$$
$$+\sum_{\alpha\sigma,\mu\mu'}\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{\mu\mu'}}{2\pi}D_\alpha^{(-)}\left(\varepsilon_{m'}-\varepsilon_{m''}\right)\langle m''|\,\rho_{\mathrm{QS}}\left(t\right)|n\rangle$$
$$-\sum_{\alpha\sigma,\mu\mu'}\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{\mu\mu'}}{2\pi}D_\alpha^{(-)}\left(\varepsilon_{n'}-\varepsilon_{n''}\right)\langle m|\,\rho_{\mathrm{QS}}\left(t\right)|n''\rangle\,, \tag{2.93}$$

其中, $\langle m'|\,d_{\mu'}=\langle m''|$, $d_{\mu'}^\dagger\,|n'\rangle=|n''\rangle$. 同理, 可以求出 $\langle m|\,B\,|n\rangle$、$\langle m|\,C\,|n\rangle$ 和 $\langle m|\,D\,|n\rangle$.

## 2.4　马尔可夫的量子主方程：忽略量子相干性

若仅考虑所研究量子系统约化密度矩阵的对角元, 即忽略该量子系统的非对角元, 则量子主方程, 即式 (2.68) 可进一步简化为

$$\frac{\mathrm{d}\rho_{\mathrm{QS}}\left(t\right)}{\mathrm{d}t}=-\sum_{\alpha\sigma,\mu\mu'}\Gamma_{\alpha\sigma}^{\mu\mu'}\left\{d_\mu^\dagger\left[f_\alpha^{(-)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)+\rho_{\mathrm{QS}}\left(t\right)\left[f_\alpha^{(+)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}\right]d_\mu^\dagger\right.$$

$$-d_{\mu}^{\dagger}\rho_{\mathrm{QS}}(t)\left[f_{\alpha}^{(+)}(-L_{\mathrm{QS}})\,d_{\mu'}\right]-\left[f_{\alpha}^{(-)}(-L_{\mathrm{QS}})\,d_{\mu'}\right]\rho_{\mathrm{QS}}(t)\,d_{\mu}^{\dagger}\Big\}. \tag{2.94}$$

因此, 约化密度矩阵 $\langle n|\,\dot{\rho}_{\mathrm{QS}}(t)\,|n\rangle$ 第一项可表示为

$$\begin{aligned}
&\langle n|\,\dot{\rho}_{\mathrm{QS}}(t)\,|n\rangle|_{01}\\
&=-\sum_{\alpha\sigma,\mu\mu'}\Gamma_{\alpha\sigma}^{\mu\mu'}\langle n|\,d_{\mu}^{\dagger}\left[f_{\alpha}^{(-)}(-L_{\mathrm{QS}})\,d_{\mu'}\right]\rho_{\mathrm{QS}}(t)\,|n\rangle\\
&=-\sum_{\alpha\sigma,\mu\mu',m}\Gamma_{\alpha\sigma}^{\mu\mu'}\langle m|\left[f_{\alpha}^{(-)}(-L_{\mathrm{QS}})\,d_{\mu'}\right]\rho_{\mathrm{QS}}(t)\,|n\rangle\\
&=-\sum_{\alpha\sigma,\mu\mu',m}\Gamma_{\alpha\sigma}^{\mu\mu'}f_{\alpha}^{(-)}(\varepsilon_{m'}-\varepsilon_{m})\,\langle m'|\,\rho_{\mathrm{QS}}(t)\,|n\rangle\,\delta_{m',n}\\
&=-\sum_{\alpha\sigma\mu m}\Gamma_{\alpha\sigma m}^{\mu}f_{\alpha}^{(-)}(\varepsilon_{n}-\varepsilon_{m})\,\langle n|\,\rho_{\mathrm{QS}}(t)\,|n\rangle,
\end{aligned} \tag{2.95}$$

其中, $\langle n|\,d_{\mu}^{\dagger}=\langle m|$, $\langle m|\,d_{\mu'}=\langle m'|\,\delta_{m',n}=\langle n|=\langle m|\,d_{\mu}$. 约化密度矩阵 $\langle n|\,\dot{\rho}_{\mathrm{QS}}(t)\,|n\rangle$ 第二项可表示为

$$\begin{aligned}
&\langle n|\,\dot{\rho}_{\mathrm{QS}}(t)\,|n\rangle|_{02}\\
&=-\sum_{\alpha\sigma,\mu\mu'}\Gamma_{\alpha\sigma}^{\mu\mu'}\langle n|\,\rho_{\mathrm{QS}}(t)\left[f_{\alpha}^{(+)}(-L_{\mathrm{QS}})\,d_{\mu'}\right]d_{\mu}^{\dagger}\,|n\rangle\\
&=-\sum_{\alpha\sigma,\mu\mu',m'}\Gamma_{\alpha\sigma}^{\mu\mu'}\langle n|\,\rho_{\mathrm{QS}}(t)\left[f_{\alpha}^{(+)}(-L_{\mathrm{QS}})\,d_{\mu'}\right]|m'\rangle\\
&=-\sum_{\alpha\sigma,\mu\mu',m'm''}\Gamma_{\alpha\sigma}^{\mu\mu'}f_{\alpha}^{(+)}(\varepsilon_{m'}-\varepsilon_{m''})\,\langle n|\,\rho_{\mathrm{QS}}(t)\,|m''\rangle\,\delta_{m'',n}\\
&=-\sum_{\alpha\sigma\mu m'}\Gamma_{\alpha\sigma m'}^{\mu}f_{\alpha}^{(+)}(\varepsilon_{m'}-\varepsilon_{n})\,\langle n|\,\rho_{\mathrm{QS}}(t)\,|n\rangle\\
&=-\sum_{\alpha\sigma\mu m}\Gamma_{\alpha\sigma m}^{\mu}f_{\alpha}^{(+)}(\varepsilon_{m}-\varepsilon_{n})\,\langle n|\,\rho_{\mathrm{QS}}(t)\,|n\rangle,
\end{aligned} \tag{2.96}$$

其中, $d_{\mu}^{\dagger}\,|n\rangle=|m'\rangle$, $d_{\mu'}\,|m'\rangle=|m''\rangle\,\delta_{m'',n}=|n\rangle$. 约化密度矩阵 $\langle n|\,\dot{\rho}_{\mathrm{QS}}(t)\,|n\rangle$ 第三项可表示为

$$\begin{aligned}
&\langle n|\,\dot{\rho}_{\mathrm{QS}}(t)\,|n\rangle|_{03}\\
&=\sum_{\alpha\sigma,\mu\mu'}\Gamma_{\alpha\sigma}^{\mu\mu'}\langle n|\,d_{\mu}^{\dagger}\rho_{\mathrm{QS}}(t)\left[f_{\alpha}^{(+)}(-L_{\mathrm{QS}})\,d_{\mu'}\right]|n\rangle\\
&=\sum_{\alpha\sigma,\mu\mu',m}\Gamma_{\alpha\sigma}^{\mu\mu'}\langle m|\,\rho_{\mathrm{QS}}(t)\left[f_{\alpha}^{(+)}(-L_{\mathrm{QS}})\,d_{\mu'}\right]|n\rangle\\
&=\sum_{\alpha\sigma,\mu\mu',mn'}\Gamma_{\alpha\sigma}^{\mu\mu'}f_{\alpha}^{(+)}(\varepsilon_{n}-\varepsilon_{n'})\,\langle m|\,\rho_{\mathrm{QS}}(t)\,|n'\rangle\,\delta_{n',m}
\end{aligned}$$

$$= \sum_{\alpha\sigma\mu m} \Gamma^{\mu}_{\alpha\sigma} f^{(+)}_{\alpha} (\varepsilon_n - \varepsilon_m) \langle m| \rho_{\mathrm{QS}} (t) |m\rangle , \tag{2.97}$$

其中, $\langle n| d^{\dagger}_{\mu} = \langle m|$, $d_{\mu'} |n\rangle = |n'\rangle \delta_{n',m} = |m\rangle = d_{\mu} |n\rangle$. 约化密度矩阵 $\langle n| \dot{\rho}_{\mathrm{QS}} (t) |n\rangle$ 第四项可表示为

$$\begin{aligned}
&\langle n| \dot{\rho}_{QS} (t) |n\rangle|_{04} \\
&= \sum_{\alpha\sigma,\mu\mu'} \Gamma^{\mu\mu'}_{\alpha\sigma} \langle n| \left[ f^{(-)}_{\alpha} (-L_{\mathrm{QS}}) d_{\mu'} \right] \rho_{\mathrm{QS}} (t) d^{\dagger}_{\mu} |n\rangle \\
&= \sum_{\alpha\sigma,\mu\mu',m'} \Gamma^{\mu\mu'}_{\alpha\sigma} \langle n| \left[ f^{(-)}_{\alpha} (-L_{\mathrm{QS}}) d_{\mu'} \right] \rho_{\mathrm{QS}} (t) |m'\rangle \\
&= \sum_{\alpha\sigma,\mu\mu',m'n''} \Gamma^{\mu\mu'}_{\alpha\sigma} f^{(-)}_{\alpha} (\varepsilon_{n''} - \varepsilon_n) \langle n''| \rho_{\mathrm{QS}} (t) |m'\rangle \delta_{n'',m'} \\
&= \sum_{\alpha\sigma\mu m'} \Gamma^{\mu}_{\alpha\sigma} f^{(-)}_{\alpha} (\varepsilon_{m'} - \varepsilon_n) \langle m'| \rho_{\mathrm{QS}} (t) |m'\rangle \\
&= \sum_{\alpha\sigma\mu m} \Gamma^{\mu}_{\alpha\sigma} f^{(-)}_{\alpha} (\varepsilon_m - \varepsilon_n) \langle m| \rho_{\mathrm{QS}} (t) |m\rangle ,
\end{aligned} \tag{2.98}$$

其中, $d^{\dagger}_{\mu} |n\rangle = |m'\rangle$, $\langle n| d_{\mu'} = \langle n''| \delta_{n'',m'} = \langle m'| = \langle n| d_{\mu}$. 利用式 (2.95) ～ 式 (2.98), 约化密度矩阵 $\langle n| \dot{\rho}_{\mathrm{QS}} (t) |n\rangle$ 可表示为

$$\begin{aligned}
\frac{\mathrm{d}P_{\mathrm{QS},n}}{\mathrm{d}t} &= \sum_{\alpha\sigma\mu m} \Gamma^{\mu}_{\alpha\sigma} \left[ f^{(+)}_{\alpha} (\varepsilon_n - \varepsilon_m) + f^{(-)}_{\alpha} (\varepsilon_m - \varepsilon_n) \right] P_{\mathrm{QS},m} \\
&\quad - \sum_{\alpha\sigma\mu m} \Gamma^{\mu}_{\alpha\sigma} \left[ f^{(+)}_{\alpha} (\varepsilon_m - \varepsilon_n) + f^{(-)}_{\alpha} (\varepsilon_n - \varepsilon_m) \right] P_{\mathrm{QS},n},
\end{aligned} \tag{2.99}$$

其中, $P_{\mathrm{QS},n} = \langle n| \rho_{\mathrm{QS}} (t) |n\rangle$. 式 (2.99) 即为式 (2.28) 描述的率方程.

## 2.5　马尔可夫的量子主方程: 忽略电子库谱函数的虚部

若忽略电子库谱函数的虚部, 即 Redfield 近似, 式 (2.74) 可以表示为

$$\int_0^{\infty} \mathrm{d}t'' \mathrm{e}^{-\mathrm{i}(\varepsilon + L_{\mathrm{QS}})t''/\hbar} = \frac{\hbar}{2} \int_{-\infty}^{\infty} \mathrm{d}\frac{t''}{\hbar} \mathrm{e}^{-\mathrm{i}(\varepsilon + L_{\mathrm{QS}})t''/\hbar} = \pi\hbar\delta (\varepsilon + L_{\mathrm{QS}}) , \tag{2.100}$$

则量子主方程, 即式 (2.68) 可进一步简化为

$$\begin{aligned}
&\frac{\mathrm{d}\rho_{\mathrm{QS}} (t)}{\mathrm{d}t} \\
&= - \sum_{\alpha\sigma,\mu\mu'} \frac{\Gamma^{\mu\mu'}_{\alpha\sigma}}{2} \left\{ d^{\dagger}_{\mu} \left[ f^{(-)}_{\alpha} (-L_{\mathrm{QS}}) d_{\mu'} \right] \rho_{\mathrm{QS}} (t) + \rho_{\mathrm{QS}} (t) \left[ f^{(+)}_{\alpha} (-L_{\mathrm{QS}}) d_{\mu'} \right] d^{\dagger}_{\mu} \right.
\end{aligned}$$

$$-d_{\mu}^{\dagger}\rho_{\mathrm{QS}}\left(t\right)\left[f_{\alpha}^{(+)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}\right]-\left[f_{\alpha}^{(-)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)d_{\mu}^{\dagger}+\mathrm{H.c.}\Big\}, \quad (2.101)$$

若定义超算符

$$A_{\alpha\mu'}^{(\pm)}=f_{\alpha}^{(\pm)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}, \quad (2.102)$$

则式 (2.101) 可进一步简写为 [8]

$$\begin{aligned}&\frac{\mathrm{d}\rho_{\mathrm{QS}}\left(t\right)}{\mathrm{d}t}\\&=-\frac{\mathrm{i}}{\hbar}\left[H_{\mathrm{QS}},\rho_{\mathrm{QS}}\left(t\right)\right]-\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2}\left[d_{\mu}^{\dagger}A_{\alpha\mu'}^{(-)}\rho_{\mathrm{QS}}\left(t\right)+\rho_{\mathrm{QS}}\left(t\right)A_{\alpha\mu'}^{(+)}d_{\mu}^{\dagger}\right.\\&\quad\left.-d_{\mu}^{\dagger}\rho_{\mathrm{QS}}\left(t\right)A_{\alpha\mu'}^{(+)}-A_{\alpha\mu'}^{(-)}\rho_{\mathrm{QS}}\left(t\right)d_{\mu}^{\dagger}+\mathrm{H.c.}\right],\end{aligned} \quad (2.103)$$

式 (2.103) 即为在马尔可夫近似和 Redfield 近似下, 开放量子系统约化密度矩阵的演化方程. 与式 (2.28) 或式 (2.99) 描述的率方程相比, 式 (2.103) 描述的量子主方程可以研究量子系统的量子相干性对其电子输运性质的影响.

## 2.6 非马尔可夫的量子主方程：相互作用绘景

一般情况下, 非马尔可夫效应对量子系统的电子实时隧穿过程有重要影响. 下面, 基于投影算符技术, 给出一种时间局域 (time-convolution-less) 的非马尔可夫量子主方程的推导过程. 在相互作用绘景中, 由式 (1.33) 可知整个开放量子系统的密度算符演化方程为

$$\frac{\partial\rho_{\mathrm{I}}\left(t\right)}{\partial t}=-\frac{\mathrm{i}}{\hbar}\left[H_{\mathrm{T,I}}\left(t\right),\rho_{\mathrm{I}}\left(t\right)\right]=L_{\mathrm{I}}\left(t\right)\rho_{\mathrm{I}}\left(t\right), \quad (2.104)$$

其中

$$L_{\mathrm{I}}\left(t\right)=-\frac{\mathrm{i}}{\hbar}\left[H_{\mathrm{T,I}}\left(t\right),\rho_{\mathrm{I}}\left(t\right)\right], \quad (2.105)$$

$$H_{\mathrm{T,I}}\left(t\right)=\mathrm{e}^{\mathrm{i}H_0t/\hbar}H_{\mathrm{T}}\mathrm{e}^{-\mathrm{i}H_0t/\hbar}=\mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t/\hbar}H_{\mathrm{T}}\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t/\hbar}, \quad (2.106)$$

$$\rho_{\mathrm{I}}\left(t\right)=\mathrm{e}^{\mathrm{i}H_0t/\hbar}\rho\left(t\right)\mathrm{e}^{-\mathrm{i}H_0t/\hbar}=\mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t/\hbar}\rho\left(t\right)\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})t/\hbar}. \quad (2.107)$$

为了推导开放量子系统约化密度矩阵的精确运动方程, 定义如下的超算符 [9]：

$$P\rho_{\mathrm{I}}\left(t\right)=\mathrm{tr}_{\mathrm{leads}}\left[\rho_{\mathrm{I}}\left(t\right)\right]\otimes\rho_{\mathrm{leads}}\equiv\rho_{\mathrm{QS,I}}\left(t\right)\otimes\rho_{\mathrm{leads}}, \quad (2.108)$$

相应地, 其互补超算符定义为

$$Q\rho_{\mathrm{I}}\left(t\right)=\left(1-P\right)\rho_{\mathrm{I}}\left(t\right)=\rho_{\mathrm{I}}\left(t\right)-P\rho_{\mathrm{I}}\left(t\right). \quad (2.109)$$

将超算符 $P$ 和 $Q$ 分别作用到式 (2.104) 可得

$$\frac{\partial}{\partial t} P\rho_{\mathrm{I}}(t) = P\frac{\partial}{\partial t}\rho_{\mathrm{I}}(t) = PL_{\mathrm{I}}(t)\rho_{\mathrm{I}}(t), \tag{2.110}$$

$$\frac{\partial}{\partial t} Q\rho_{\mathrm{I}}(t) = Q\frac{\partial}{\partial t}\rho_{\mathrm{I}}(t) = QL_{\mathrm{I}}(t)\rho_{\mathrm{I}}(t), \tag{2.111}$$

利用超算符 $P$ 和 $Q$ 的性质 $P+Q=1$, 可将式 (2.110) 和式 (2.111) 写为

$$\frac{\partial}{\partial t} P\rho_{\mathrm{I}}(t) = PL_{\mathrm{I}}(t)P\rho_{\mathrm{I}}(t) + PL_{\mathrm{I}}(t)Q\rho_{\mathrm{I}}(t), \tag{2.112}$$

$$\frac{\partial}{\partial t} Q\rho_{\mathrm{I}}(t) = QL_{\mathrm{I}}(t)P\rho_{\mathrm{I}}(t) + QL_{\mathrm{I}}(t)Q\rho_{\mathrm{I}}(t). \tag{2.113}$$

若初始时刻 $t_0$ 的密度矩阵为 $\rho_{\mathrm{I}}(t_0)$, 则式 (2.113) 的形式解可以写为

$$Q\rho_{\mathrm{I}}(t) = G_{\leftarrow}(t,t_0)Q\rho_{\mathrm{I}}(t_0) + \int_{t_0}^{t} \mathrm{d}s G_{\leftarrow}(t,s)QL_{\mathrm{I}}(s)P\rho_{\mathrm{I}}(s), \tag{2.114}$$

其中

$$G_{\leftarrow}(t,s) \equiv T_{\leftarrow}\exp\left[\int_{s}^{t} \mathrm{d}s' QL_{\mathrm{I}}(s')\right], \tag{2.115}$$

为开放量子系统的传播子, $T_{\leftarrow}$ 为时序算符, 即它将超算符乘积中的时间变量从右到左依次增加, 推导见附录 C, 该传播子满足

$$\frac{\partial}{\partial t} G_{\leftarrow}(t,s) = QL_{\mathrm{I}}(t)G_{\leftarrow}(t,s), \tag{2.116}$$

对于初始条件, 有

$$G_{\leftarrow}(s,s) = 1, \tag{2.117}$$

同样, 利用超算符 $P$ 和 $Q$ 的性质 $P+Q=1$, 可将开放量子系统的密度算符表示为

$$\rho_{\mathrm{I}}(s) = G_{\rightarrow}(t,s)(P+Q)\rho_{\mathrm{I}}(t), \tag{2.118}$$

其中

$$G_{\rightarrow}(t,s) \equiv T_{\rightarrow}\exp\left[-\int_{s}^{t} \mathrm{d}s' L_{\mathrm{I}}(s')\right], \tag{2.119}$$

为开放量子系统的向后传播子, 即开放量子系统时间演化算符的逆. 这里, $T_{\rightarrow}$ 为反时序算符, 它将超算符乘积中的时间变量从左到右依次增加. 将式 (2.118) 代入式 (2.114) 可得

$$Q\rho_{\mathrm{I}}(t) = G_{\leftarrow}(t,t_0)Q\rho_{\mathrm{I}}(t_0) + \int_{t_0}^{t} \mathrm{d}s G_{\leftarrow}(t,s)QL_{\mathrm{I}}(s)PG_{\rightarrow}(t,s)(P+Q)\rho_{\mathrm{I}}(t). \tag{2.120}$$

若定义超算符

$$\sum(t)=\int_{t_0}^{t}\mathrm{d}sG_{\leftarrow}(t,s)\,QL_{\mathrm{I}}(s)\,PG_{\rightarrow}(t,s)\,, \tag{2.121}$$

则式 (2.120) 可以表示为

$$\left[1-\sum(t)\right]Q\rho_{\mathrm{I}}(t)=G_{\leftarrow}(t,t_0)\,Q\rho_{\mathrm{I}}(t_0)+\sum(t)P\rho_{\mathrm{I}}(t)\,. \tag{2.122}$$

求解式 (2.122) 可得

$$Q\rho_{\mathrm{I}}(t)=\left[1-\sum(t)\right]^{-1}G_{\leftarrow}(t,t_0)\,Q\rho_{\mathrm{I}}(t_0)+\left[1-\sum(t)\right]^{-1}\sum(t)P\rho_{\mathrm{I}}(t)\,. \tag{2.123}$$

这里需要说明的是, 超算符 $\sum(t)$ 包含传播子 $G_{\leftarrow}$ 和 $G_{\rightarrow}$, 因而, 其没有一个确定的时序. 此外, 当量子系统与电极之间的耦合强度比较大时, 或者时间间隔 $t-t_0$ 很大时, 式 (2.122) 将可能不能唯一求解 $Q\rho_{\mathrm{I}}(t)$, 因而 $\left[1-\sum(t)\right]$ 的逆将不存在.

为了推导一个时间局域的量子主方程, 将式 (2.123) 代入式 (2.112) 可得

$$\begin{aligned}\frac{\partial}{\partial t}P\rho_{\mathrm{I}}(t)&=\left\{PL_{\mathrm{I}}(t)+PL_{\mathrm{I}}(t)\left[1-\sum(t)\right]^{-1}\sum(t)\right\}P\rho_{\mathrm{I}}(t)\\&\quad+PL_{\mathrm{I}}(t)\left[1-\sum(t)\right]^{-1}G_{\leftarrow}(t,t_0)\,Q\rho_{\mathrm{I}}(t_0)\\&=PL_{\mathrm{I}}(t)\,\frac{1-\sum(t)+\sum(t)}{1-\sum(t)}P\rho_{\mathrm{I}}(t)\\&\quad+PL_{\mathrm{I}}(t)\left[1-\sum(t)\right]^{-1}G_{\leftarrow}(t,t_0)\,Q\rho_{\mathrm{I}}(t_0)\,,\end{aligned} \tag{2.124}$$

即

$$\frac{\partial}{\partial t}P\rho_{\mathrm{I}}(t)=K(t)\,P\rho_{\mathrm{I}}(t)+I(t)\,Q\rho_{\mathrm{I}}(t_0)\,, \tag{2.125}$$

其中

$$K(t)=PL_{\mathrm{I}}(t)\left[1-\sum(t)\right]^{-1}P, \tag{2.126}$$

$$I(t)=PL_{\mathrm{I}}(t)\left[1-\sum(t)\right]^{-1}G_{\leftarrow}(t,t_0)\,Q. \tag{2.127}$$

在式 (2.125) 的推导中, 已经利用了超算符的性质 $P^2=P$ 和 $Q^2=Q$. 若在初始时刻 $t_0$, 开放量子系统的密度算符可以表示为量子系统的密度算符 $\rho_{\mathrm{QS,I}}(t_0)$ 和电子库密度算符 $\rho_{\mathrm{leads}}$ 的直积, 即

$$\rho_{\mathrm{I}}(t_0)=\rho_{\mathrm{QS,I}}(t_0)\otimes\rho_{\mathrm{leads}}, \tag{2.128}$$

则有

$$P\rho_{\mathrm{I}}(t_0)=\mathrm{tr}_{\mathrm{leads}}\left[\rho_{\mathrm{I}}(t_0)\right]\otimes\rho_{\mathrm{leads}}\equiv\rho_{\mathrm{QS,I}}(t_0)\otimes\rho_{\mathrm{leads}}=\rho_{\mathrm{I}}(t_0)\,, \tag{2.129}$$

因而

$$Q\rho_{\mathrm{I}}(t_0)=(1-P)\,\rho_{\mathrm{I}}(t_0)=\rho_{\mathrm{I}}(t_0)-P\rho_{\mathrm{I}}(t_0)=0. \tag{2.130}$$

将式 (2.130) 代入式 (2.125) 可得

$$\frac{\partial}{\partial t}P\rho_{\mathrm{I}}(t)=K(t)\,P\rho_{\mathrm{I}}(t)\,. \tag{2.131}$$

为了确定式 (2.131) 中 $K(t)$ 的阶数, 将 $\left[1-\sum(t)\right]^{-1}$ 展成级数形式

$$\left[1-\sum(t)\right]^{-1}=\sum_{n=0}^{\infty}\left[\sum(t)\right]^{n}, \tag{2.132}$$

将式 (2.132) 代入式 (2.126) 可得

$$K(t)=\sum_{n=0}^{\infty}PL_{\mathrm{I}}(t)\left[\sum(t)\right]^{n}P. \tag{2.133}$$

由于超算符 $\sum(t)$ 也可以展成级数形式

$$\sum(t)=\sum_{n=1}^{\infty}\sum_{n}(t), \tag{2.134}$$

将式 (2.134) 代入式 (2.133) 可得超算符 $K(t)$ 的前四阶分别为

$$K_1(t)=PL_{\mathrm{I}}(t)\,P, \tag{2.135}$$

$$K_2(t)=PL_{\mathrm{I}}(t)\sum_{1}(t)\,P, \tag{2.136}$$

$$K_3(t)=PL_{\mathrm{I}}(t)\left\{\left[\sum_{1}(t)\right]^{2}+\sum_{2}(t)\right\}P, \tag{2.137}$$

$$K_4(t)=PL_{\mathrm{I}}(t)\left\{\left[\sum_{1}(t)\right]^{3}+\sum_{1}(t)\sum_{2}(t)+\sum_{2}(t)\sum_{1}(t)+\sum_{3}(t)\right\}P. \tag{2.138}$$

由式 (2.115) 和式 (2.119) 可得

$$\begin{aligned}G_{\leftarrow}(t,t_0)&\equiv T_{\leftarrow}\exp\left[\int_{t_0}^{t}\mathrm{d}t_1QL_{\mathrm{I}}(t_1)\right]\\&=1+\frac{1}{1!}\int_{t_0}^{t}\mathrm{d}t_1QL_{\mathrm{I}}(t_1)+\frac{1}{2!}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t}\mathrm{d}t_2T_{\leftarrow}QL_{\mathrm{I}}(t_1)\,QL_{\mathrm{I}}(t_2)+\cdots\\&=1+\int_{t_0}^{t}\mathrm{d}t_1QL_{\mathrm{I}}(t_1)+\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2QL_{\mathrm{I}}(t_1)\,QL_{\mathrm{I}}(t_2)+\cdots,\end{aligned} \tag{2.139}$$

$$
\begin{aligned}
G_{\rightarrow}(t,t_0) &\equiv T_{\rightarrow}\exp\left[-\int_{t_0}^{t}\mathrm{d}t_1 L_{\mathrm{I}}(t_1)\right] \\
&= 1-\int_{t_0}^{t}\mathrm{d}t_1 L_{\mathrm{I}}(t_1)+\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t}\mathrm{d}t_2 T_{\rightarrow}L_{\mathrm{I}}(t_1)\,L_{\mathrm{I}}(t_2)+\cdots \\
&= 1-\int_{t_0}^{t}\mathrm{d}t_1 L_{\mathrm{I}}(t_1)+\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2 L_{\mathrm{I}}(t_2)\,L_{\mathrm{I}}(t_1)+\cdots,
\end{aligned}
\tag{2.140}
$$

将式 (2.139) 和式 (2.140) 代入式 (2.133) 可得超算符 $\sum_{n}(t)$ 的前三阶表达式为

$$
\sum_{1}(t)=\int_{t_0}^{t}\mathrm{d}t_1 QL_{\mathrm{I}}(t_1)\,P, \tag{2.141}
$$

$$
\sum_{2}(t)=\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\left[QL_{\mathrm{I}}(t_1)\,L_{\mathrm{I}}(t_2)\,P-L_{\mathrm{I}}(t_2)\,PL(t_1)\right], \tag{2.142}
$$

$$
\begin{aligned}
\sum_{3}(t)=\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\,&\left[-QL_{\mathrm{I}}(t_1)\,L_{\mathrm{I}}(t_3)\,PL_{\mathrm{I}}(t_2)\right. \\
&-QL_{\mathrm{I}}(t_2)\,L_{\mathrm{I}}(t_3)\,PL_{\mathrm{I}}(t_1)+QL_{\mathrm{I}}(t_1)\,QL_{\mathrm{I}}(t_2)\,L_{\mathrm{I}}(t_3)\,P \\
&\left.+L_{\mathrm{I}}(t_3)\,PL_{\mathrm{I}}(t_2)\,L_{\mathrm{I}}(t_1)\right].
\end{aligned}
\tag{2.143}
$$

计算过程见附录 D. 利用超算符的性质 $PQ=QP=0$, 可得

$$
\left[\sum_{1}(t)\right]^{2}=\left[\sum_{1}(t)\right]^{3}=0, \tag{2.144}
$$

$$
\begin{aligned}
&\sum_{1}(t)\sum_{2}(t) \\
&=\int_{t_0}^{t}\mathrm{d}t_3\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2 QL_{\mathrm{I}}(t_3)\,P\left[QL_{\mathrm{I}}(t_1)\,L_{\mathrm{I}}(t_2)\,P-L_{\mathrm{I}}(t_2)\,PL_{\mathrm{I}}(t_1)\right]=0,
\end{aligned}
\tag{2.145}
$$

$$
\begin{aligned}
\sum_{2}(t)\sum_{1}(t)=-\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\,&\left[L_{\mathrm{I}}(t_3)\,PL_{\mathrm{I}}(t_2)\,L_{\mathrm{I}}(t_1)\,P\right. \\
&\left.+L_{\mathrm{I}}(t_3)\,PL_{\mathrm{I}}(t_1)\,L_{\mathrm{I}}(t_2)\,P+L_{\mathrm{I}}(t_2)\,PL_{\mathrm{I}}(t_1)\,L_{\mathrm{I}}(t_3)\,P\right],
\end{aligned}
\tag{2.146}
$$

计算过程见附录 D. 基于式 (2.141) ∼ 式 (2.146), 并考虑到量子系统与电极的隧穿耦合项为量子系统产生 (湮灭) 算符和电极湮灭 (产生) 算符的线性组合, 超算符 $K(t)$ 的前四阶项可以分别表示为

$$
K_1(t)=PL_{\mathrm{I}}(t)\,P=0, \tag{2.147}
$$

$$K_2(t) = \int_{t_0}^{t} \mathrm{d}t_1 P L_\mathrm{I}(t) Q L_\mathrm{I}(t_1) PP = \int_{t_0}^{t} \mathrm{d}t_1 P L_\mathrm{I}(t) L_\mathrm{I}(t_1) P, \tag{2.148}$$

$$\begin{aligned} K_3(t) &= P L_\mathrm{I}(t) \left\{ \left[ \sum_1 (t) \right]^2 + \sum_2 (t) \right\} P = P L_\mathrm{I}(t) \sum_2 (t) P \\ &= \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 P L_\mathrm{I}(t) \left[ L_\mathrm{I}(t_1) L_\mathrm{I}(t_2) P - L_\mathrm{I}(t_2) P L(t_1) \right] P = 0, \end{aligned} \tag{2.149}$$

$$\begin{aligned} K_4(t) &= P L_\mathrm{I}(t) \left\{ \sum_2 (t) \sum_1 (t) + \sum_3 (t) \right\} P \\ &= \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \int_{t_0}^{t_2} \mathrm{d}t_3 \left[ P L_\mathrm{I}(t) L_\mathrm{I}(t_1) L_\mathrm{I}(t_2) L_\mathrm{I}(t_3) P \right. \\ &\quad - P L_\mathrm{I}(t) L_\mathrm{I}(t_1) P L_\mathrm{I}(t_2) L_\mathrm{I}(t_3) P - P L_\mathrm{I}(t) L_\mathrm{I}(t_2) P L_\mathrm{I}(t_1) L_\mathrm{I}(t_3) P \\ &\quad \left. - P L_\mathrm{I}(t) L_\mathrm{I}(t_3) P L_\mathrm{I}(t_1) L_\mathrm{I}(t_2) P \right]. \end{aligned} \tag{2.150}$$

因而, 在二阶和四阶近似下, 时间局域的非马尔可夫量子主方程可以分别表示为

$$\frac{\partial}{\partial t} P \rho_\mathrm{I}(t) = K_2(t) P \rho_\mathrm{I}(t) = \int_{t_0}^{t} \mathrm{d}t_1 P L_\mathrm{I}(t) L_\mathrm{I}(t_1) P \rho_\mathrm{I}(t), \tag{2.151}$$

$$\begin{aligned} \frac{\partial}{\partial t} P \rho_\mathrm{I}(t) &= \left[ K_2(t) + K_4(t) \right] P \rho_\mathrm{I}(t) \\ &= \int_{t_0}^{t} \mathrm{d}t_1 P L_\mathrm{I}(t) L_\mathrm{I}(t_1) P \rho_\mathrm{I}(t) \\ &\quad + \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \int_{t_0}^{t_2} \mathrm{d}t_3 \left[ P L_\mathrm{I}(t) L_\mathrm{I}(t_1) L_\mathrm{I}(t_2) L_\mathrm{I}(t_3) P \right. \\ &\quad - P L_\mathrm{I}(t) L_\mathrm{I}(t_1) P L_\mathrm{I}(t_2) L_\mathrm{I}(t_3) P - P L_\mathrm{I}(t) L_\mathrm{I}(t_2) P L_\mathrm{I}(t_1) L_\mathrm{I}(t_3) P \\ &\quad \left. - P L_\mathrm{I}(t) L_\mathrm{I}(t_3) P L_\mathrm{I}(t_1) L_\mathrm{I}(t_2) P \right]. \end{aligned} \tag{2.152}$$

在本章中, 只考虑在二阶近似下, 即电子顺序隧穿极限下, 时间局域的非马尔可夫量子主方程. 在四阶近似下, 即电子共隧穿辅助顺序隧穿极限下, 时间局域的非马尔可夫量子主方程将在第 4 章重点讨论.

## 2.7 非马尔可夫的量子主方程: 薛定谔绘景

在本小节中, 将相互作用绘景中的二阶时间局域量子主方程变换到薛定谔绘景中. 利用超算符 $P$ 和 $L_\mathrm{I}(t)$ 的定义, 可将式 (2.151) 左边和右边分别写为

$$\frac{\partial}{\partial t} P \rho_\mathrm{I}(t) = \frac{\partial}{\partial t} \mathrm{tr}_\mathrm{leads} \left[ \rho_\mathrm{I}(t) \right] \otimes \rho_\mathrm{leads} = \frac{\partial \rho_{\mathrm{QS,I}}(t)}{\partial t} \otimes \rho_\mathrm{leads}, \tag{2.153}$$

$$
\begin{aligned}
&\int_{t_0}^{t} \mathrm{d}t_1 P L_{\mathrm{I}}(t) L_{\mathrm{I}}(t_1) P \rho_{\mathrm{I}}(t) \\
&= \int_{t_0}^{t} \mathrm{d}t_1 P L_{\mathrm{I}}(t) L_{\mathrm{I}}(t_1) \mathrm{tr}_{\mathrm{leads}}[\rho_{\mathrm{I}}(t)] \otimes \rho_{\mathrm{leads}} \\
&= -\frac{1}{\hbar^2}\int_{t_0}^{t} \mathrm{d}t_1 P [H_{\mathrm{T,I}}(t), [H_{\mathrm{T,I}}(t_1), \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}}]] \\
&= -\frac{1}{\hbar^2}\int_{t_0}^{t} \mathrm{d}t_1 \mathrm{tr}_{\mathrm{leads}} [H_{\mathrm{T,I}}(t), [H_{\mathrm{T,I}}(t_1), \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}}]] \otimes \rho_{\mathrm{leads}},
\end{aligned} \tag{2.154}
$$

即式 (2.151) 可以重新写为

$$
\frac{\partial \rho_{\mathrm{QS,I}}(t)}{\partial t} = -\frac{1}{\hbar^2}\int_{t_0}^{t} \mathrm{d}t_1 \mathrm{tr}_{\mathrm{leads}} [H_{\mathrm{T,I}}(t), [H_{\mathrm{T,I}}(t_1), \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}}]], \tag{2.155}
$$

将式 (2.155) 右边展开可得

$$
\begin{aligned}
\frac{\partial \rho_{\mathrm{QS,I}}(t)}{\partial t} = &-\frac{1}{\hbar^2}\int_{t_0}^{t} \mathrm{d}t_1 \mathrm{tr}_{\mathrm{leads}} [\rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t_1) H_{\mathrm{T,I}}(t)] \\
&-\frac{1}{\hbar^2}\int_{t_0}^{t} \mathrm{d}t_1 \mathrm{tr}_{\mathrm{leads}} [H_{\mathrm{T,I}}(t) H_{\mathrm{T,I}}(t_1) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}}] \\
&+\frac{1}{\hbar^2}\int_{t_0}^{t} \mathrm{d}t_1 \mathrm{tr}_{\mathrm{leads}} [H_{\mathrm{T,I}}(t) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t_1)] \\
&+\frac{1}{\hbar^2}\int_{t_0}^{t} \mathrm{d}t_1 \mathrm{tr}_{\mathrm{leads}} [H_{\mathrm{T,I}}(t_1) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t)].
\end{aligned} \tag{2.156}
$$

将式 (2.156) 变换到薛定谔绘景中可得

$$
\begin{aligned}
&\frac{\mathrm{d}\rho_{\mathrm{QS}}(t)}{\mathrm{d}t} \\
&= -\frac{\mathrm{i}}{\hbar}[H_{\mathrm{QS}}, \rho_{\mathrm{QS}}(t)] - \frac{1}{\hbar^2}\int_{t_0}^{t} \mathrm{d}t_1 \mathrm{tr}_{\mathrm{leads}} \\
&\quad \times \left[\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}})t/\hbar} \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t_1) H_{\mathrm{T,I}}(t) \mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}})t/\hbar}\right] \\
&\quad - \frac{1}{\hbar^2}\int_{t_0}^{t} \mathrm{d}t_1 \mathrm{tr}_{\mathrm{leads}} \left[\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}})t/\hbar} H_{\mathrm{T,I}}(t) H_{\mathrm{T,I}}(t_1) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} \mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}})t/\hbar}\right] \\
&\quad + \frac{1}{\hbar^2}\int_{t_0}^{t} \mathrm{d}t_1 \mathrm{tr}_{\mathrm{leads}} \left[\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}})t/\hbar} H_{\mathrm{T,I}}(t) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t_1) \mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}})t/\hbar}\right] \\
&\quad + \frac{1}{\hbar^2}\int_{t_0}^{t} \mathrm{d}t_1 \mathrm{tr}_{\mathrm{leads}} \left[\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}})t/\hbar} H_{\mathrm{T,I}}(t_1) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t) \mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}})t/\hbar}\right],
\end{aligned} \tag{2.157}
$$

将式 (2.157) 中的相互作用绘景算符展开可得

$$\begin{aligned}
&\frac{\mathrm{d}\rho_{\mathrm{QS}}(t)}{\mathrm{d}t}\\
=&-\frac{\mathrm{i}}{\hbar}\left[H_{\mathrm{QS}},\rho_{\mathrm{QS}}(t)\right]-\frac{1}{\hbar^2}\int_{t_0}^{t}\mathrm{d}t_1\mathrm{tr}_{\mathrm{leads}}\\
&\times\left[\rho_{\mathrm{QS}}(t)\otimes\rho_{\mathrm{leads}}\mathrm{e}^{-\mathrm{i}(H_{QS}+H_{\mathrm{leads}})(t-t_1)/\hbar}H_{\mathrm{T}}\mathrm{e}^{\mathrm{i}(H_{QS}+H_{\mathrm{leads}})(t-t_1)/\hbar}H_{\mathrm{T}}\right]\\
&-\frac{1}{\hbar^2}\int_{t_0}^{t}\mathrm{d}t_1\mathrm{tr}_{\mathrm{leads}}\left[H_{\mathrm{T}}\mathrm{e}^{-\mathrm{i}(H_{QS}+H_{\mathrm{leads}})(t-t_1)/\hbar}H_{\mathrm{T}}\mathrm{e}^{\mathrm{i}(H_{QS}+H_{\mathrm{leads}})(t-t_1)/\hbar}\rho_{\mathrm{QS}}(t)\otimes\rho_{\mathrm{leads}}\right]\\
&+\frac{1}{\hbar^2}\int_{t_0}^{t}\mathrm{d}t_1\mathrm{tr}_{\mathrm{leads}}\left[H_{\mathrm{T}}\rho_{\mathrm{QS}}(t)\otimes\rho_{\mathrm{leads}}\mathrm{e}^{-\mathrm{i}(H_{QS}+H_{\mathrm{leads}})(t-t_1)/\hbar}H_{\mathrm{T}}\mathrm{e}^{\mathrm{i}(H_{QS}+H_{\mathrm{leads}})(t-t_1)/\hbar}\right]\\
&+\frac{1}{\hbar^2}\int_{t_0}^{t}\mathrm{d}t_1\mathrm{tr}_{\mathrm{leads}}\left[\mathrm{e}^{-\mathrm{i}(H_{QS}+H_{\mathrm{leads}})(t-t_1)/\hbar}H_{\mathrm{T}}\mathrm{e}^{\mathrm{i}(H_{QS}+H_{\mathrm{leads}})(t-t_1)/\hbar}\rho_{\mathrm{QS}}(t)\otimes\rho_{\mathrm{leads}}H_{\mathrm{T}}\right],
\end{aligned}\tag{2.158}$$

与描述马尔可夫量子主方程的式 (2.49) 相比, 上式右边中的开放量子系统的约化密度算符 $\rho_{\mathrm{QS}}(t)$ 是时间定域的, 不再依赖于该系统先前时刻的时间. 利用式 (2.64)~式 (2.67), 时间局域的非马尔可夫量子主方程可表示为

$$\frac{\mathrm{d}\rho_{\mathrm{QS}}(t)}{\mathrm{d}t}=-\frac{\mathrm{i}}{\hbar}\left[H_{\mathrm{QS}},\rho_{\mathrm{QS}}(t)\right]+\left(A_{\mathrm{Non}}+B_{\mathrm{Non}}+C_{\mathrm{Non}}+D_{\mathrm{Non}}\right),\tag{2.159}$$

其中

$$\begin{aligned}
A_{\mathrm{Non}}=&-\sum_{\alpha\boldsymbol{k}\sigma}\sum_{\mu\mu'}\frac{\left|t_{\alpha\boldsymbol{k}\sigma}\right|_{\mu\mu'}^2}{\hbar^2}\int_{t_0}^{t}\mathrm{d}t_1 f_{\alpha}^{(-)}(\varepsilon_{\alpha\boldsymbol{k}\sigma})\,d_{\mu}^{\dagger}\left[\mathrm{e}^{-\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}+L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu'}\right]\rho_{\mathrm{QS}}(t)\\
&-\sum_{\alpha\boldsymbol{k}\sigma}\sum_{\mu\mu'}\frac{\left|t_{\alpha\boldsymbol{k}\sigma}\right|_{\mu\mu'}^2}{\hbar^2}\int_{t_0}^{t}\mathrm{d}t_1 f_{\alpha}^{(-)}(\varepsilon_{\alpha\boldsymbol{k}\sigma})\,\rho_{\mathrm{QS}}(t)\left[\mathrm{e}^{\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}-L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu'}^{\dagger}\right]d_{\mu},
\end{aligned}\tag{2.160}$$

$$\begin{aligned}
B_{\mathrm{Non}}=&-\sum_{\alpha\boldsymbol{k}\sigma}\sum_{\mu\mu'}\frac{\left|t_{\alpha\boldsymbol{k}\sigma}\right|_{\mu\mu'}^2}{\hbar^2}\int_{t_0}^{t}\mathrm{d}t_1 f_{\alpha}^{(+)}(\varepsilon_{\alpha\boldsymbol{k}\sigma})\,d_{\mu}\left[\mathrm{e}^{\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}-L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu'}^{\dagger}\right]\rho_{\mathrm{QS}}(t)\\
&-\sum_{\alpha\boldsymbol{k}\sigma}\sum_{\mu\mu'}\frac{\left|t_{\alpha\boldsymbol{k}\sigma}\right|_{\mu\mu'}^2}{\hbar^2}\int_{t_0}^{t}\mathrm{d}t_1 f_{\alpha}^{(+)}(\varepsilon_{\alpha\boldsymbol{k}\sigma})\,\rho_{\mathrm{QS}}(t)\left[\mathrm{e}^{-\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}+L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu'}\right]d_{\mu}^{\dagger},
\end{aligned}\tag{2.161}$$

$$C_{\mathrm{Non}}=\sum_{\alpha\boldsymbol{k}\sigma}\sum_{\mu\mu'}\frac{\left|t_{\alpha\boldsymbol{k}\sigma}\right|_{\mu\mu'}^2}{\hbar^2}\int_{t_0}^{t}\mathrm{d}t_1 f_{\alpha}^{(+)}(\varepsilon_{\alpha\boldsymbol{k}\sigma})\,d_{\mu}^{\dagger}\rho_{\mathrm{QS}}(t)\left[\mathrm{e}^{-\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}+L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu'}\right]$$

$$+\sum_{\alpha\boldsymbol{k}\sigma}\sum_{\mu\mu'}\frac{\left|t_{\alpha\boldsymbol{k}\sigma}\right|^2_{\mu\mu'}}{\hbar^2}\int_{t_0}^{t}\mathrm{d}t_1 f_\alpha^{(+)}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\right)\left[\mathrm{e}^{\mathrm{i}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}-L_{\mathrm{QS}}\right)(t-t_1)/\hbar}d_{\mu'}^{\dagger}\right]\rho_{\mathrm{QS}}\left(t\right)d_\mu, \tag{2.162}$$

$$D_{\mathrm{Non}}=\sum_{\alpha\boldsymbol{k}\sigma}\sum_{\mu\mu'}\frac{\left|t_{\alpha\boldsymbol{k}\sigma}\right|^2_{\mu\mu'}}{\hbar^2}\int_{t_0}^{t}\mathrm{d}t_1 f_\alpha^{(-)}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\right)d_\mu\rho_{\mathrm{QS}}\left(t\right)\left[\mathrm{e}^{\mathrm{i}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}-L_{\mathrm{QS}}\right)(t-t_1)/\hbar}d_{\mu'}^{\dagger}\right]$$
$$+\sum_{\alpha\boldsymbol{k}\sigma}\sum_{\mu\mu'}\frac{\left|t_{\alpha\boldsymbol{k}\sigma}\right|^2_{\mu\mu'}}{\hbar^2}\int_{t_0}^{t}\mathrm{d}t_1 f_\alpha^{(-)}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\right)\left[\mathrm{e}^{-\mathrm{i}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}+L_{\mathrm{QS}}\right)(t-t_1)/\hbar}d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)d_\mu^{\dagger}, \tag{2.163}$$

下面考虑一种特殊的情况, 即对于类似于式 (2.17) 描述的微扰项缓慢打开的情形, 为了保持 $t$ 为有限值, 选取 $\eta\to 0^+$, 此时 $t_0\to-\infty$, 上面式 (2.160) ~ 式 (2.163) 中关于 $t_1$ 的积分可以改写为

$$\begin{aligned}&\int_{t_0}^{t}\mathrm{d}t_1\mathrm{e}^{\pm\mathrm{i}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}\right)(t-t_1)/\hbar}\\
=&\lim_{\eta\to0^+}\int_{-\infty}^{t}\mathrm{d}t_1\mathrm{e}^{\pm\mathrm{i}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}\right)(t-t_1)/\hbar}\mathrm{e}^{\eta(t+t_1)}\\
=&\lim_{\eta\to0^+}\int_{-\infty}^{t}\mathrm{d}t_1\mathrm{e}^{\pm\mathrm{i}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}\mp\mathrm{i}\eta\hbar\right)t/\hbar}\mathrm{e}^{\mp\mathrm{i}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}\pm\mathrm{i}\eta\hbar\right)t_1/\hbar},\end{aligned} \tag{2.164}$$

对式 (2.164) 积分可得

$$\begin{aligned}&\lim_{\eta\to0^+}\int_{-\infty}^{t}\mathrm{d}t_1\mathrm{e}^{\pm\mathrm{i}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}\right)(t-t_1)/\hbar}\mathrm{e}^{\eta(t+t_1)}\\
=&\lim_{\eta\to0^+}\frac{\mathrm{e}^{\pm\mathrm{i}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}\mp\mathrm{i}\eta\hbar\right)t/\hbar}\mathrm{e}^{\mp\mathrm{i}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}\pm\mathrm{i}\eta\hbar\right)t/\hbar}}{\mp\mathrm{i}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}\pm\mathrm{i}\eta\hbar\right)/\hbar}=\lim_{\eta\to0^+}\frac{\pm\mathrm{i}\hbar\mathrm{e}^{\eta t}}{\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}\pm\mathrm{i}\eta\hbar}\\
=&\lim_{\eta\to0^+}\frac{\pm\mathrm{i}\hbar\mathrm{e}^{\eta t}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}\mp\mathrm{i}\eta\hbar\right)}{\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}\right)^2+\left(\eta\hbar\right)^2}\\
=&\lim_{\eta\to0^+}\frac{\pm\mathrm{i}\hbar\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}\right)}{\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}\right)^2+\left(\eta\hbar\right)^2}+\hbar\lim_{\eta\hbar\to0^+}\frac{\eta\hbar}{\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}\right)^2+\left(\eta\hbar\right)^2}\\
=&\pm\mathrm{i}\hbar\mathrm{P}\frac{1}{\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}}+\hbar\pi\delta\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}\right).\end{aligned} \tag{2.165}$$

将式 (2.165) 代入式 (2.160) ~ 式 (2.163) 可得

$$A_{\mathrm{Non}}=-\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2}\left\{d_\mu^{\dagger}\left[f_\alpha^{(-)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)+\rho_{\mathrm{QS}}\left(t\right)\left[f_\alpha^{(-)}\left(L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]d_\mu\right\}$$

$$
+\mathrm{i}\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2\pi}\left\{d_{\mu}^{\dagger}\left[D_{\alpha}^{(-)}\left(L_{\mathrm{QS}}\right)d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)-\rho_{\mathrm{QS}}\left(t\right)\left[D_{\alpha}^{(-)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]d_{\mu}\right\},
\tag{2.166}
$$

$$
\begin{aligned}
B_{\mathrm{Non}}=&-\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2}\left\{\rho_{\mathrm{QS}}\left(t\right)\left[f_{\alpha}^{(+)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}\right]d_{\mu}^{\dagger}+d_{\mu}\left[f_{\alpha}^{(+)}\left(L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]\rho_{\mathrm{QS}}\left(t\right)\right\}\\
&+\mathrm{i}\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2\pi}\left\{\rho_{\mathrm{QS}}\left(t\right)\left[D_{\alpha}^{(+)}\left(L_{\mathrm{QS}}\right)d_{\mu'}\right]d_{\mu}^{\dagger}-d_{\mu}\left[D_{\alpha}^{(+)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]\rho_{\mathrm{QS}}\left(t\right)\right\},
\end{aligned}
\tag{2.167}
$$

$$
\begin{aligned}
C_{\mathrm{Non}}=&\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2}\left\{d_{\mu}^{\dagger}\rho_{\mathrm{QS}}\left(t\right)\left[f_{\alpha}^{(+)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}\right]+\left[f_{\alpha}^{(+)}\left(L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]\rho_{\mathrm{QS}}\left(t\right)d_{\mu}\right\}\\
&-\mathrm{i}\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2\pi}\left\{d_{\mu}^{\dagger}\rho_{\mathrm{QS}}\left(t\right)\left[D_{\alpha}^{(+)}\left(L_{\mathrm{QS}}\right)d_{\mu'}\right]-\left[D_{\alpha}^{(+)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]\rho_{\mathrm{QS}}\left(t\right)d_{\mu}\right\},
\end{aligned}
\tag{2.168}
$$

$$
\begin{aligned}
D_{\mathrm{Non}}=&\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2}\left\{\left[f_{\alpha}^{(-)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)d_{\mu}^{\dagger}+d_{\mu}\rho_{\mathrm{QS}}\left(t\right)\left[f_{\alpha}^{(-)}\left(L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]\right\}\\
&-\mathrm{i}\sum_{\alpha\sigma,\mu\mu'}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2\pi}\left\{\left[D_{\alpha}^{(-)}\left(L_{\mathrm{QS}}\right)d_{\mu'}\right]\rho_{\mathrm{QS}}\left(t\right)d_{\mu}^{\dagger}-d_{\mu}\rho_{\mathrm{QS}}\left(t\right)\left[D_{\alpha}^{(-)}\left(-L_{\mathrm{QS}}\right)d_{\mu'}^{\dagger}\right]\right\},
\end{aligned}
\tag{2.169}
$$

其中, $\Gamma_{\alpha\sigma}^{\mu\mu'}=2\pi\rho_{\alpha\sigma}\left|t_{\alpha\sigma}\right|_{\mu\mu'}^{2}\Big/\hbar$, $D_{\alpha}^{(\pm)}\left(\mp L_{\mathrm{QS}}\right)$ 的定义见式 (2.83) ~ 式 (2.86). 这里需要说明的是, 虽然在微扰项缓慢打开情形下描述时间定域的非马尔可夫量子主方程的式 (2.159) 与描述马尔可夫量子主方程的式 (2.68) 相同, 但是它们所用的近似不同. 例如, 在式 (2.68) 的推导中使用了马尔可夫近似, 且其初始时刻选取为 $t_0=0$, 即积分限为 $\int_{0}^{\infty}\mathrm{d}t_1$; 而式 (2.159) 仅假设微扰项缓慢打开的情形, 相应的积分限为 $\int_{-\infty}^{t}\mathrm{d}t_1$. 在一般情况下, 式 (2.159) 描述的非马尔可夫量子主方程, 若选择初始时刻为 $t_0=0$, 相比式 (2.68) 描述的马尔可夫量子主方程, 式 (2.165) 中的第二项将不同, 即

$$
\begin{aligned}
&\int_{t_0=0}^{t}\mathrm{d}t_1\mathrm{e}^{\pm\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}})(t-t_1)/\hbar}\\
=&\frac{\mathrm{e}^{\pm\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}})t/\hbar}\mathrm{e}^{\mp\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}})t_1/\hbar}}{\mp\mathrm{i}\left(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}\right)/\hbar}=\frac{\pm\mathrm{i}\hbar\mathrm{e}^{\pm\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}})t/\hbar}\ \mathrm{e}^{\mp\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}})t_1/\hbar}\Big|_{0}^{t}}{\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}}\\
=&\frac{\pm\mathrm{i}\hbar\left[1-\mathrm{e}^{\pm\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}})t/\hbar}\right]}{\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}}=\pm\mathrm{i}\hbar\mathrm{P}\frac{1}{\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}}\mp\mathrm{i}\hbar\mathrm{P}\frac{\mathrm{e}^{\pm\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}})t/\hbar}}{\varepsilon_{\alpha\boldsymbol{k}\sigma}\mp L_{\mathrm{QS}}}.
\end{aligned}
\tag{2.170}
$$

# 参 考 文 献

[1] Bruus H, Flensberg K. Many-body Quantum Theory in Condensed Matter Physics. Oxford: Oxford University Press, 2004: 87, 88.

[2] Elste F, Timm C. Theory for transport through a single magnetic molecule: Endohedral N@$C_{60}$. Phys. Rev. B, 2005, 71: 155403.

[3] Timm C, Elste F. Spin amplification, reading, and writing in transport through anisotropic magnetic molecules. Phys. Rev. B, 2006, 73: 235304.

[4] Blum K. Density Matrix Theory and Applications. 3rd ed. Dordrecht: Springer, 2012: 155-168.

[5] Timm C. Tunneling through molecules and quantum dots: Master-equation approaches. Phys. Rev. B, 2008, 77: 195416.

[6] 曾谨言. 量子力学卷Ⅱ. 5 版. 北京：科学出版社, 2014: 82.

[7] 吴崇试. 数学物理方法. 2 版. 北京：北京大学出版社, 2003：第 7 章, 第 8 章.

[8] Li X Q, Luo J Y, Yang Y G, et al. Quantum master-equation approach to quantum transport through mesoscopic systems. Phys. Rev. B, 2005, 71: 205304.

[9] Breuer H P, Petruccione F. The Theory of Open Quantum Systems. Oxford: Oxford University Press, 2002: Chap. 9.

# 第 3 章　二阶非马尔可夫的电子计数统计理论

在本章中, 将基于时间局域的二阶非马尔可夫量子主方程推导其对应的粒子数分辨的量子主方程, 并给出计算电流前四阶累积矩的计算方法, 并以一个与两个电极弱耦合的量子点为例给出其计算流程.

## 3.1　粒子数分辨的二阶非马尔可夫量子主方程

在一个开放量子系统中, 完全描述该体系的电子输运过程, 需要记录电子从源极 (左电极) 隧穿到该系统, 再从该系统隧穿到漏极 (右电极) 的电子数. 因而, 需要将电极的希尔伯特空间做如下分类 [1]：首先, 将没有电子隧穿到源极和没有电子隧穿到漏极的子空间记为 $B^{(0)} \equiv \mathrm{span}\left\{|\Psi_{\mathrm{L}}\rangle \otimes |\Psi_{\mathrm{R}}\rangle\right\}$, 它由两个孤立电极的所有多粒子态的直积组成. 若有 $n_{\mathrm{L}}$ 个电子隧穿到源极同时有 $n_{\mathrm{R}}$ 个电子隧穿到漏极, 相应的两个电极的希尔伯特子空间记为 $B^{(n_{\mathrm{L}},n_{\mathrm{R}})}$ $(n_{\mathrm{L}} = 0, 1, 2, \cdots; n_{\mathrm{R}} = 0, 1, 2, \cdots)$. 因而, 两个电极的整个希尔伯特子空间可以表示成 $B = \oplus_{n_{\mathrm{L}},n_{\mathrm{R}}} B^{(n_{\mathrm{L}},n_{\mathrm{R}})}$. 此时, 式 (2.159) 关于对两个电极的整个希尔伯特空间平均需要替换为对其子空间的平均

$$\frac{\mathrm{d}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)}{\mathrm{d}t} = -\frac{\mathrm{i}}{\hbar}\left[H_{\mathrm{QS}}, \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\right] + A_{\mathrm{con}} + B_{\mathrm{con}} + C_{\mathrm{con}} + D_{\mathrm{con}}, \tag{3.1}$$

其中

$$\begin{aligned}&A_{\mathrm{con}}\\ =&-\frac{1}{\hbar^2}\int_{t_0}^{t}\mathrm{d}t_1\mathrm{tr}_{B^{(n_{\mathrm{L}},n_{\mathrm{R}})}}\Big[\rho_{\mathrm{QS}}(t)\otimes\rho_{\mathrm{leads}}\mathrm{e}^{-\mathrm{i}\left(H_{\mathrm{QS}}+H_{\mathrm{leads}}\right)(t-t_1)/\hbar}H_{\mathrm{T}}\mathrm{e}^{\mathrm{i}\left(H_{\mathrm{QS}}+H_{\mathrm{leads}}\right)(t-t_1)/\hbar}H_{\mathrm{T}}\Big],\end{aligned} \tag{3.2}$$

$$\begin{aligned}&B_{\mathrm{con}}\\ =&-\frac{1}{\hbar^2}\int_{t_0}^{t}\mathrm{d}t_1\mathrm{tr}_{B^{(n_{\mathrm{L}},n_{\mathrm{R}})}}\Big[H_{\mathrm{T}}\mathrm{e}^{-\mathrm{i}\left(H_{\mathrm{QS}}+H_{\mathrm{leads}}\right)(t-t_1)/\hbar}H_{\mathrm{T}}\mathrm{e}^{\mathrm{i}\left(H_{\mathrm{QS}}+H_{\mathrm{leads}}\right)(t-t_1)/\hbar}\rho_{\mathrm{QS}}(t)\otimes\rho_{\mathrm{leads}}\Big],\end{aligned} \tag{3.3}$$

$$\begin{aligned}&C_{\mathrm{con}}\\ =&\frac{1}{\hbar^2}\int_{t_0}^{t}\mathrm{d}t_1\mathrm{tr}_{B^{(n_{\mathrm{L}},n_{\mathrm{R}})}}\Big[H_{\mathrm{T}}\rho_{\mathrm{QS}}(t)\otimes\rho_{\mathrm{leads}}\mathrm{e}^{-\mathrm{i}\left(H_{\mathrm{QS}}+H_{\mathrm{leads}}\right)(t-t_1)/\hbar}H_{\mathrm{T}}\mathrm{e}^{\mathrm{i}\left(H_{\mathrm{QS}}+H_{\mathrm{leads}}\right)(t-t_1)/\hbar}\Big],\end{aligned} \tag{3.4}$$

$$
\begin{aligned}
&D_{\mathrm{con}}\\
=&\frac{1}{\hbar^2}\int_{t_0}^{t}\mathrm{d}t_1\mathrm{tr}_{B^{(n_\mathrm{L},n_\mathrm{R})}}\Big[\mathrm{e}^{-\mathrm{i}\left(H_{\mathrm{QS}}+H_{\mathrm{leads}}\right)(t-t_1)/\hbar}H_{\mathrm{T}}\mathrm{e}^{\mathrm{i}\left(H_{\mathrm{QS}}+H_{\mathrm{leads}}\right)(t-t_1)/\hbar}\rho_{\mathrm{QS}}\left(t\right)\otimes\rho_{\mathrm{leads}}H_{\mathrm{T}}\Big],
\end{aligned}\tag{3.5}
$$

其中, $\rho_{\mathrm{QS}}^{(n_\mathrm{L},n_\mathrm{R})}\left(t\right)\equiv\mathrm{tr}_{B^{(n_\mathrm{L},n_\mathrm{R})}}\left[\rho\left(t\right)\right]$ 是开放量子系统的条件性约化密度矩阵, 其约束条件为到 $t$ 时刻有 $n_\mathrm{L}$ 个电子隧穿到源极同时有 $n_\mathrm{R}$ 个电子隧穿到漏极. 另外, 引入假设

$$
\rho\left(t\right)=\sum_{n_\mathrm{L},n_\mathrm{R}}\rho_{\mathrm{QS}}^{(n_\mathrm{L},n_\mathrm{R})}\left(t\right)\otimes\rho_{\mathrm{leads}}^{(n_\mathrm{L},n_\mathrm{R})},\tag{3.6}
$$

替代传统的玻恩近似 $\rho\left(t\right)=\rho_{\mathrm{QS}}\left(t\right)\otimes\rho_{\mathrm{leads}}$, 其中 $\rho_{\mathrm{leads}}^{(n_\mathrm{L},n_\mathrm{R})}$ 表示有 $n_\mathrm{L}$ 个电子隧穿到源极同时有 $n_\mathrm{R}$ 个电子隧穿到漏极时的电极库密度算符. 将式 (2.4) 代入式 (3.2) 可得

$$
\begin{aligned}
A_{\mathrm{con}}=&-\frac{1}{\hbar^2}\sum_{\alpha\mu\boldsymbol{k}\sigma}\sum_{\alpha'\mu'\boldsymbol{k}'\sigma'}\mathrm{tr}_{B^{(n_\mathrm{L},n_\mathrm{R})}}\int_{t_0}^{t}\mathrm{d}t_1\sum_{m_\mathrm{L},m_\mathrm{R}}\rho_{\mathrm{QS}}^{(m_\mathrm{L},m_\mathrm{R})}\left(t\right)\otimes\rho_{\mathrm{leads}}^{(m_\mathrm{L},m_\mathrm{R})}\\
&\times\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})(t-t_1)/\hbar}\left(t_{\alpha\mu\boldsymbol{k}\sigma}d_\mu^\dagger a_{\alpha\boldsymbol{k}\sigma}+t_{\alpha\mu\boldsymbol{k}\sigma}^*a_{\alpha\boldsymbol{k}\sigma}^\dagger d_\mu\right)\\
&\times\mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})(t-t_1)/\hbar}\left(t_{\alpha'\mu'\boldsymbol{k}'\sigma'}d_{\mu'}^\dagger a_{\alpha'\boldsymbol{k}'\sigma'}+t_{\alpha'\mu'\boldsymbol{k}'\sigma'}^*a_{\alpha'\boldsymbol{k}'\sigma'}^\dagger d_{\mu'}\right),
\end{aligned}\tag{3.7}
$$

式 (3.7) 的非零项可表示为

$$
\begin{aligned}
A_{\mathrm{con}}=&-\frac{1}{\hbar^2}\sum_{\alpha\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2\int_{t_0}^{t}\mathrm{d}t_1\left\langle B^{(n_\mathrm{L},n_\mathrm{R})}\right|\sum_{m_\mathrm{L},m_\mathrm{R}}W_{m_\mathrm{L},m_\mathrm{R}}\left|B^{(m_\mathrm{L},m_\mathrm{R})}\right\rangle\left\langle B^{(m_\mathrm{L},m_\mathrm{R})}\right|\\
&\otimes\rho_{\mathrm{QS}}^{(m_\mathrm{L},m_\mathrm{R})}\left(t\right)\Big[\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})(t-t_1)/\hbar}d_\mu^\dagger a_{\alpha\boldsymbol{k}\sigma}\mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})(t-t_1)/\hbar}a_{\alpha\boldsymbol{k}\sigma}^\dagger d_{\mu'}\\
&+\mathrm{e}^{-\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})(t-t_1)/\hbar}a_{\alpha\boldsymbol{k}\sigma}^\dagger d_\mu\mathrm{e}^{\mathrm{i}(H_{\mathrm{QS}}+H_{\mathrm{leads}})(t-t_1)/\hbar}d_{\mu'}^\dagger a_{\alpha\boldsymbol{k}\sigma}\Big]\left|B^{(n_\mathrm{L},n_\mathrm{R})}\right\rangle,
\end{aligned}\tag{3.8}
$$

利用不同电子数的希尔伯特子空间之间正交, 即

$$
\left\langle B^{(n_\mathrm{L},n_\mathrm{R})}\right|\left|B^{(m_\mathrm{L},m_\mathrm{R})}\right\rangle=\delta_{n_\mathrm{L},m_\mathrm{L}}\delta_{n_\mathrm{R},m_\mathrm{R}},\tag{3.9}
$$

可将式 (3.8) 重写为

$$
\begin{aligned}
A_{\mathrm{con}}=&-\frac{1}{\hbar^2}\sum_{\alpha\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2\int_{t_0}^{t}\mathrm{d}t_1\rho_{\mathrm{QS}}^{(n_\mathrm{L},n_\mathrm{R})}\left(t\right)\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}(t-t_1)/\hbar}d_\mu^\dagger\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_1)/\hbar}d_{\mu'}\\
&\times\mathrm{tr}_{B^{(n_\mathrm{L},n_\mathrm{R})}}\left[\rho_{\mathrm{leads}}^{(n_\mathrm{L},n_\mathrm{R})}\mathrm{e}^{-\mathrm{i}H_{\mathrm{leads}}(t-t_1)/\hbar}a_{\alpha\boldsymbol{k}\sigma}\mathrm{e}^{\mathrm{i}H_{\mathrm{leads}}(t-t_1)/\hbar}a_{\alpha\boldsymbol{k}\sigma}^\dagger\right]\\
&-\frac{1}{\hbar^2}\sum_{\alpha\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2\int_{t_0}^{t}\mathrm{d}t_1\rho_{\mathrm{QS}}^{(n_\mathrm{L},n_\mathrm{R})}\left(t\right)\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}(t-t_1)/\hbar}d_\mu\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_1)/\hbar}d_{\mu'}^\dagger
\end{aligned}
$$

$$\times \operatorname{tr}_{B^{(n_{\mathrm{L}},n_{\mathrm{R}})}}\left[\rho_{\mathrm{leads}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}\mathrm{e}^{-\mathrm{i}H_{\mathrm{leads}}(t-t_1)/\hbar}a_{\alpha\boldsymbol{k}\sigma}^{\dagger}\mathrm{e}^{\mathrm{i}H_{\mathrm{leads}}(t-t_1)/\hbar}a_{\alpha\boldsymbol{k}\sigma}\right], \tag{3.10}$$

由于式 (3.10) 中

$$\mathrm{e}^{-\mathrm{i}H_{\mathrm{leads}}(t-t_1)/\hbar}a_{\alpha\boldsymbol{k}\sigma}^{\dagger}\mathrm{e}^{\mathrm{i}H_{\mathrm{leads}}(t-t_1)/\hbar}=\mathrm{e}^{-\mathrm{i}\varepsilon_{\alpha\boldsymbol{k}\sigma}(t-t_1)/\hbar}a_{\alpha\boldsymbol{k}\sigma}^{\dagger}, \tag{3.11}$$

$$\mathrm{e}^{-\mathrm{i}H_{\mathrm{leads}}(t-t_1)/\hbar}a_{\alpha\boldsymbol{k}\sigma}\mathrm{e}^{\mathrm{i}H_{\mathrm{leads}}(t-t_1)/\hbar}=\mathrm{e}^{\mathrm{i}\varepsilon_{\alpha\boldsymbol{k}\sigma}(t-t_1)/\hbar}a_{\alpha\boldsymbol{k}\sigma}, \tag{3.12}$$

因而, 式 (3.10) 可以简化为

$$\begin{aligned}
A_{\mathrm{con}}=&-\frac{1}{\hbar^2}\sum_{\alpha\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2\operatorname{tr}_{B^{(n_{\mathrm{L}},n_{\mathrm{R}})}}\left[\rho_{\mathrm{leads}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}a_{\alpha\boldsymbol{k}\sigma}a_{\alpha\boldsymbol{k}\sigma}^{\dagger}\right]\\
&\times\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\left[\int_{t_0}^{t}\mathrm{d}t_1\mathrm{e}^{\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}-L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu}^{\dagger}\right]d_{\mu'}\\
&-\frac{1}{\hbar^2}\sum_{\alpha\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2\operatorname{tr}_{B^{(n_{\mathrm{L}},n_{\mathrm{R}})}}\left[\rho_{\mathrm{leads}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}a_{\alpha\boldsymbol{k}\sigma}^{\dagger}a_{\alpha\boldsymbol{k}\sigma}\right]\\
&\times\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\left[\int_{t_0}^{t}\mathrm{d}t_1\mathrm{e}^{-\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}+L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu}\right]d_{\mu'}^{\dagger},
\end{aligned}\tag{3.13}$$

需要指出的是, 对于一个封闭的电子输运电路, 隧穿到漏极 (右电极) 的电子将通过外电路返回到源极 (左电极). 特别是, 电子库的快速弛豫过程将其很快恢复到化学势确定的定域热平衡态. 因而, 电子库密度矩阵 $\rho_{\mathrm{leads}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}$、$\rho_{\mathrm{leads}}^{(n_{\mathrm{L}},n_{\mathrm{R}}\pm1)}$、$\rho_{\mathrm{leads}}^{(n_{\mathrm{L}}\pm1,n_{\mathrm{R}})}$ 应该用 $\rho_{\mathrm{leads}}$ 代替. 所以, 式 (3.13) 可进一步表示为

$$\begin{aligned}
A_{\mathrm{con}}=&-\frac{1}{\hbar^2}\sum_{\alpha\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\left[\int_{t_0}^{t}\mathrm{d}t_1 f_{\alpha}^{(-)}(\varepsilon_{\alpha\boldsymbol{k}\sigma})\,\mathrm{e}^{\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}-L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu'}^{\dagger}\right]d_{\mu}\\
&-\frac{1}{\hbar^2}\sum_{\alpha\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\left[\int_{t_0}^{t}\mathrm{d}t_1 f_{\alpha}^{(+)}(\varepsilon_{\alpha\boldsymbol{k}\sigma})\,\mathrm{e}^{-\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}+L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu'}\right]d_{\mu}^{\dagger},
\end{aligned}\tag{3.14}$$

其中, $f_{\alpha}^{(+)}(\varepsilon_{\alpha\boldsymbol{k}\sigma})=f_{\alpha}(\varepsilon_{\alpha\boldsymbol{k}\sigma})$, $f_{\alpha}^{(-)}(\varepsilon_{\alpha\boldsymbol{k}\sigma})=1-f_{\alpha}(\varepsilon_{\alpha\boldsymbol{k}\sigma})$. 对于式 (3.3), 同理可得

$$\begin{aligned}
B_{\mathrm{con}}=&-\frac{1}{\hbar^2}\sum_{\alpha\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2 d_{\mu}^{\dagger}\left[\int_{t_0}^{t}\mathrm{d}t_1 f_{\alpha}^{(-)}(\varepsilon_{\alpha\boldsymbol{k}\sigma})\,\mathrm{e}^{-\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}+L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu'}\right]\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\\
&-\frac{1}{\hbar^2}\sum_{\alpha\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2 d_{\mu}\left[\int_{t_0}^{t}\mathrm{d}t_1 f_{\alpha}^{(+)}(\varepsilon_{\alpha\boldsymbol{k}\sigma})\,\mathrm{e}^{\mathrm{i}(\varepsilon_{\alpha\boldsymbol{k}\sigma}-L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu'}^{\dagger}\right]\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t).
\end{aligned}\tag{3.15}$$

对于式 (3.4), 可将其表示为

$$C_{\mathrm{con}}=\frac{1}{\hbar^2}\sum_{\alpha\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2\int_{t_0}^{t}\mathrm{d}t_1$$

$$
\begin{aligned}
&\times \left\langle B^{(n_{\rm L},n_{\rm R})}\right| d_\mu^\dagger a_{\alpha\boldsymbol{k}\sigma} \sum_{m_{\rm L},m_{\rm R}} W_{m_{\rm L},m_{\rm R}} \left|B^{(m_{\rm L},m_{\rm R})}\right\rangle\!\left\langle B^{(m_{\rm L},m_{\rm R})}\right| \\
&\otimes \rho_{\rm QS}^{(m_{\rm L},m_{\rm R})}(t)\,\mathrm{e}^{-\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar} a_{\alpha\boldsymbol{k}\sigma}^\dagger d_{\mu'} \mathrm{e}^{\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar} \left|B^{(n_{\rm L},n_{\rm R})}\right\rangle \\
&+ \frac{1}{\hbar^2} \sum_{\alpha\mu\mu'\boldsymbol{k}\sigma} \left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2 \int_{t_0}^{t} \mathrm{d}t_1 \\
&\times \left\langle B^{(n_{\rm L},n_{\rm R})}\right| a_{\alpha\boldsymbol{k}\sigma}^\dagger d_\mu \sum_{m_{\rm L},m_{\rm R}} W_{m_{\rm L},m_{\rm R}} \left|B^{(m_{\rm L},m_{\rm R})}\right\rangle \left\langle B^{(m_{\rm L},m_{\rm R})}\right| \\
&\otimes \rho_{\rm QS}^{(m_{\rm L},m_{\rm R})}(t)\,\mathrm{e}^{-\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar} d_{\mu'}^\dagger a_{\alpha\boldsymbol{k}\sigma} \mathrm{e}^{\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar} \left|B^{(n_{\rm L},n_{\rm R})}\right\rangle,
\end{aligned}
\tag{3.16}
$$

在式 (3.16) 中, 对电子库的希尔伯特子空间求迹时, 态矢量 $\left\langle B^{(n_{\rm L},n_{\rm R})}\right|$ 和其密度算符之间有电极库的产生或湮灭算符, 因此, 需要将其进一步写为

$$
\begin{aligned}
&C_{\rm con} \\
=&\frac{1}{\hbar^2} \sum_{\mu\mu'\boldsymbol{k}\sigma} \left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2 \int_{t_0}^{t} \mathrm{d}t_1 \left\langle B^{(n_{\rm L},n_{\rm R})}\right| d_\mu^\dagger a_{{\rm L}\boldsymbol{k}\sigma} \sum_{m_{\rm L},m_{\rm R}} W_{m_{\rm L},m_{\rm R}} \left|B^{(m_{\rm L},m_{\rm R})}\right\rangle\!\left\langle B^{(m_{\rm L},m_{\rm R})}\right| \\
&\otimes \rho_{\rm QS}^{(m_{\rm L},m_{\rm R})}(t)\,\mathrm{e}^{-\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar} a_{{\rm L}\boldsymbol{k}\sigma}^\dagger d_{\mu'} \mathrm{e}^{\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar} \left|B^{(n_{\rm L},n_{\rm R})}\right\rangle \\
&+ \frac{1}{\hbar^2} \sum_{\mu\mu'\boldsymbol{k}\sigma} \left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2 \int_{t_0}^{t} \mathrm{d}t_1 \left\langle B^{(n_{\rm L},n_{\rm R})}\right| d_\mu^\dagger a_{{\rm R}\boldsymbol{k}\sigma} \sum_{m_{\rm L},m_{\rm R}} W_{m_{\rm L},m_{\rm R}} \left|B^{(m_{\rm L},m_{\rm R})}\right\rangle\!\left\langle B^{(m_{\rm L},m_{\rm R})}\right| \\
&\otimes \rho_{\rm QS}^{(m_{\rm L},m_{\rm R})}(t)\,\mathrm{e}^{-\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar} a_{{\rm R}\boldsymbol{k}\sigma}^\dagger d_{\mu'} \mathrm{e}^{\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar} \left|B^{(n_{\rm L},n_{\rm R})}\right\rangle \\
&+ \frac{1}{\hbar^2} \sum_{\alpha\mu\mu'\boldsymbol{k}\sigma} \left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2 \int_{t_0}^{t} \mathrm{d}t_1 \left\langle B^{(n_{\rm L},n_{\rm R})}\right| a_{{\rm L}\boldsymbol{k}\sigma}^\dagger d_\mu \sum_{m_{\rm L},m_{\rm R}} W_{m_{\rm L},m_{\rm R}} \left|B^{(m_{\rm L},m_{\rm R})}\right\rangle\!\left\langle B^{(m_{\rm L},m_{\rm R})}\right| \\
&\otimes \rho_{\rm QS}^{(m_{\rm L},m_{\rm R})}(t)\,\mathrm{e}^{-\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar} d_{\mu'}^\dagger a_{{\rm L}\boldsymbol{k}\sigma} \mathrm{e}^{\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar} \left|B^{(n_{\rm L},n_{\rm R})}\right\rangle \\
&+ \frac{1}{\hbar^2} \sum_{\alpha\mu\mu'\boldsymbol{k}\sigma} \left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2 \int_{t_0}^{t} \mathrm{d}t_1 \left\langle B^{(n_{\rm L},n_{\rm R})}\right| a_{{\rm R}\boldsymbol{k}\sigma}^\dagger d_\mu \sum_{m_{\rm L},m_{\rm R}} W_{m_{\rm L},m_{\rm R}} \left|B^{(m_{\rm L},m_{\rm R})}\right\rangle\!\left\langle B^{(m_{\rm L},m_{\rm R})}\right| \\
&\otimes \rho_{\rm QS}^{(m_{\rm L},m_{\rm R})}(t)\,\mathrm{e}^{-\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar} d_{\mu'}^\dagger a_{{\rm R}\boldsymbol{k}\sigma} \mathrm{e}^{\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar} \left|B^{(n_{\rm L},n_{\rm R})}\right\rangle,
\end{aligned}
\tag{3.17}
$$

由于希尔伯特子空间在电子的产生或湮灭算符作用下, 有

$$
\left\langle B^{(n_{\rm L},n_{\rm R})}\right| a_{{\rm L}\boldsymbol{k}\sigma} = \left\langle B^{(n_{\rm L}+1,n_{\rm R})}\right| a_{{\rm L}\boldsymbol{k}\sigma}, \quad \left\langle B^{(n_{\rm L},n_{\rm R})}\right| a_{{\rm R}\boldsymbol{k}\sigma} = \left\langle B^{(n_{\rm L},n_{\rm R}+1)}\right| a_{{\rm R}\boldsymbol{k}\sigma},
\tag{3.18}
$$

$$
\left\langle B^{(n_{\rm L},n_{\rm R})}\right| a_{{\rm L}\boldsymbol{k}\sigma}^\dagger = \left\langle B^{(n_{\rm L}-1,n_{\rm R})}\right| a_{{\rm L}\boldsymbol{k}\sigma}^\dagger, \quad \left\langle B^{(n_{\rm L},n_{\rm R})}\right| a_{{\rm L}\boldsymbol{k}\sigma}^\dagger = \left\langle B^{(n_{\rm L}-1,n_{\rm R})}\right| a_{{\rm L}\boldsymbol{k}\sigma}^\dagger,
\tag{3.19}
$$

因而式 (3.17) 可表示为

$$
\begin{aligned}
C_{\rm con}=\frac{1}{\hbar^2}\sum_{\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2\int_{t_0}^{t}\mathrm{d}t_1\mathrm{tr}_{B^{(n_{\rm L},n_{\rm R})}}&\Big[d_\mu^\dagger a_{{\rm L}\boldsymbol{k}\sigma}\rho_{\rm leads}^{(n_{\rm L}+1,n_{\rm R})}\otimes\rho_{\rm QS}^{(n_{\rm L}+1,n_{\rm R})}(t)\\
&\times \mathrm{e}^{-\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar}a_{{\rm L}\boldsymbol{k}\sigma}^\dagger d_{\mu'}\mathrm{e}^{\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar}\\
&+d_\mu^\dagger a_{{\rm R}\boldsymbol{k}\sigma}\rho_{\rm leads}^{(n_{\rm L},n_{\rm R}+1)}\otimes\rho_{\rm QS}^{(n_{\rm L},n_{\rm R}+1)}(t)\\
&\times \mathrm{e}^{-\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar}a_{{\rm R}\boldsymbol{k}\sigma}^\dagger d_{\mu'}\mathrm{e}^{\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar}\\
&+a_{{\rm L}\boldsymbol{k}\sigma}^\dagger d_\mu\rho_{\rm leads}^{(n_{\rm L}-1,n_{\rm R})}\otimes\rho_{\rm QS}^{(n_{\rm L}-1,n_{\rm R})}(t)\\
&\times \mathrm{e}^{-\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar}d_{\mu'}^\dagger a_{{\rm L}\boldsymbol{k}\sigma}\mathrm{e}^{\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar}\\
&+a_{{\rm R}\boldsymbol{k}\sigma}^\dagger d_\mu\rho_{\rm leads}^{(n_{\rm L},n_{\rm R}-1)}\otimes\rho_{\rm QS}^{(n_{\rm L},n_{\rm R}-1)}(t)\\
&\times \mathrm{e}^{-\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar}d_{\mu'}^\dagger a_{{\rm R}\boldsymbol{k}\sigma}\mathrm{e}^{\mathrm{i}(H_{\rm QS}+H_{\rm leads})(t-t_1)/\hbar}\Big],
\end{aligned}
\tag{3.20}
$$

上式计算过程中利用了不同电子数的希尔伯特子空间之间的正交性. 将式 (3.20) 进一步整理可得

$$
\begin{aligned}
&C_{\rm con}\\
=&\frac{1}{\hbar^2}\sum_{\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2\int_{t_0}^{t}\mathrm{d}t_1\mathrm{tr}_{B^{(n_{\rm L},n_{\rm R})}}\Big[\mathrm{e}^{-\mathrm{i}H_{\rm leads}(t-t_1)/\hbar}a_{{\rm L}\boldsymbol{k}\sigma}^\dagger\mathrm{e}^{\mathrm{i}H_{\rm leads}(t-t_1)/\hbar}a_{{\rm L}\boldsymbol{k}\sigma}\rho_{\rm leads}^{(n_{\rm L}+1,n_{\rm R})}\Big]\\
&\times d_\mu^\dagger\rho_{\rm QS}^{(n_{\rm L}+1,n_{\rm R})}(t)\,\mathrm{e}^{-\mathrm{i}H_{\rm QS}(t-t_1)/\hbar}d_{\mu'}\mathrm{e}^{\mathrm{i}H_{\rm QS}(t-t_1)/\hbar}\\
&+\frac{1}{\hbar^2}\sum_{\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2\int_{t_0}^{t}\mathrm{d}t_1\mathrm{tr}_{B^{(n_{\rm L},n_{\rm R})}}\Big[\mathrm{e}^{-\mathrm{i}H_{\rm leads}(t-t_1)/\hbar}a_{{\rm R}\boldsymbol{k}\sigma}^\dagger\mathrm{e}^{\mathrm{i}H_{\rm leads}(t-t_1)/\hbar}a_{{\rm R}\boldsymbol{k}\sigma}\rho_{\rm leads}^{(n_{\rm L},n_{\rm R}+1)}\Big]\\
&\times d_\mu^\dagger\rho_{\rm QS}^{(n_{\rm L},n_{\rm R}+1)}(t)\,\mathrm{e}^{-\mathrm{i}H_{\rm QS}(t-t_1)/\hbar}d_{\mu'}\mathrm{e}^{\mathrm{i}H_{\rm QS}(t-t_1)/\hbar}\\
&+\frac{1}{\hbar^2}\sum_{\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2\int_{t_0}^{t}\mathrm{d}t_1\mathrm{tr}_{B^{(n_{\rm L},n_{\rm R})}}\Big[\mathrm{e}^{-\mathrm{i}H_{\rm leads}(t-t_1)/\hbar}a_{{\rm L}\boldsymbol{k}\sigma}\mathrm{e}^{\mathrm{i}H_{\rm leads}(t-t_1)/\hbar}a_{{\rm L}\boldsymbol{k}\sigma}^\dagger\rho_{\rm leads}^{(n_{\rm L}-1,n_{\rm R})}\Big]\\
&\times d_\mu\rho_{\rm QS}^{(n_{\rm L}-1,n_{\rm R})}(t)\,\mathrm{e}^{-\mathrm{i}H_{\rm QS}(t-t_1)/\hbar}d_{\mu'}^\dagger\mathrm{e}^{\mathrm{i}H_{\rm QS}(t-t_1)/\hbar}\\
&+\frac{1}{\hbar^2}\sum_{\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2\int_{t_0}^{t}\mathrm{d}t_1\mathrm{tr}_{B^{(n_{\rm L},n_{\rm R})}}\Big[\mathrm{e}^{-\mathrm{i}H_{\rm leads}(t-t_1)/\hbar}a_{{\rm R}\boldsymbol{k}\sigma}\mathrm{e}^{\mathrm{i}H_{\rm leads}(t-t_1)/\hbar}a_{{\rm R}\boldsymbol{k}\sigma}^\dagger\rho_{\rm leads}^{(n_{\rm L},n_{\rm R}-1)}\Big]\\
&\times d_\mu\rho_{\rm QS}^{(n_{\rm L},n_{\rm R}-1)}(t)\,\mathrm{e}^{-\mathrm{i}H_{\rm QS}(t-t_1)/\hbar}d_{\mu'}^\dagger\mathrm{e}^{\mathrm{i}H_{\rm QS}(t-t_1)/\hbar},
\end{aligned}
\tag{3.21}
$$

将式 (3.11) 和式 (3.12) 代入式 (3.21), 并将 $\rho_{\rm leads}^{(n_{\rm L},n_{\rm R}\pm1)}$ 和 $\rho_{\rm leads}^{(n_{\rm L}\pm1,n_{\rm R})}$ 用 $\rho_{\rm leads}$ 代替可得

$$
C_{\rm con}=\frac{1}{\hbar^2}\sum_{\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2 d_\mu^\dagger\rho_{\rm QS}^{(n_{\rm L}+1,n_{\rm R})}(t)\left[\int_{t_0}^{t}\mathrm{d}t_1 f_{\rm L}^{(+)}(\varepsilon_{{\rm L}\boldsymbol{k}\sigma})\,\mathrm{e}^{-\mathrm{i}(\varepsilon_{{\rm L}\boldsymbol{k}\sigma}+L_{\rm QS})(t-t_1)/\hbar}d_{\mu'}\right]
$$

$$
\begin{aligned}
&+\frac{1}{\hbar^2}\sum_{\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2 d_\mu^\dagger\rho_{\mathrm{QS}}^{(n_\mathrm{L},n_\mathrm{R}+1)}(t)\left[\int_{t_0}^{t}\mathrm{d}t_1 f_\mathrm{R}^{(+)}(\varepsilon_{\mathrm{R}\boldsymbol{k}\sigma})\,\mathrm{e}^{-\mathrm{i}(\varepsilon_{\mathrm{R}\boldsymbol{k}\sigma}+L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu'}\right]\\
&+\frac{1}{\hbar^2}\sum_{\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2 d_\mu\rho_{\mathrm{QS}}^{(n_\mathrm{L}-1,n_\mathrm{R})}(t)\left[\int_{t_0}^{t}\mathrm{d}t_1 f_\mathrm{L}^{(-)}(\varepsilon_{\mathrm{L}\boldsymbol{k}\sigma})\,\mathrm{e}^{\mathrm{i}(\varepsilon_{\mathrm{L}\boldsymbol{k}\sigma}-L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu'}^\dagger\right]\\
&+\frac{1}{\hbar^2}\sum_{\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2 d_\mu\rho_{\mathrm{QS}}^{(n_\mathrm{L},n_\mathrm{R}-1)}(t)\left[\int_{t_0}^{t}\mathrm{d}t_1 f_\mathrm{R}^{(-)}(\varepsilon_{\mathrm{R}\boldsymbol{k}\sigma})\,\mathrm{e}^{\mathrm{i}(\varepsilon_{\mathrm{R}\boldsymbol{k}\sigma}-L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu'}^\dagger\right],
\end{aligned}
\tag{3.22}
$$

同理可将式 (3.5) 表示为

$$
\begin{aligned}
&D_{\mathrm{con}}\\
&=\frac{1}{\hbar^2}\sum_{\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2\left[\int_{t_0}^{t}\mathrm{d}t_1 f_\mathrm{L}^{(+)}(\varepsilon_{\mathrm{L}\boldsymbol{k}\sigma})\,\mathrm{e}^{\mathrm{i}(\varepsilon_{\mathrm{L}\boldsymbol{k}\sigma}-L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu'}^\dagger\right]\rho_{\mathrm{QS}}^{(n_\mathrm{L}+1,n_\mathrm{R})}(t)\,d_\mu\\
&\quad+\frac{1}{\hbar^2}\sum_{\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2\left[\int_{t_0}^{t}\mathrm{d}t_1 f_\mathrm{R}^{(+)}(\varepsilon_{\mathrm{R}\boldsymbol{k}\sigma})\,\mathrm{e}^{\mathrm{i}(\varepsilon_{\mathrm{R}\boldsymbol{k}\sigma}-L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu'}^\dagger\right]\rho_{\mathrm{QS}}^{(n_\mathrm{L},n_\mathrm{R}+1)}(t)\,d_\mu\\
&\quad+\frac{1}{\hbar^2}\sum_{\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2\left[\int_{t_0}^{t}\mathrm{d}t_1 f_\mathrm{L}^{(-)}(\varepsilon_{\mathrm{L}\boldsymbol{k}\sigma})\,\mathrm{e}^{-\mathrm{i}(\varepsilon_{\mathrm{L}\boldsymbol{k}\sigma}+L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu'}\right]\rho_{\mathrm{QS}}^{(n_\mathrm{L}-1,n_\mathrm{R})}(t)\,d_\mu^\dagger\\
&\quad+\frac{1}{\hbar^2}\sum_{\mu\mu'\boldsymbol{k}\sigma}\left|t_{\alpha\boldsymbol{k}\sigma}^{\mu\mu'}\right|^2\left[\int_{t_0}^{t}\mathrm{d}t_1 f_\mathrm{R}^{(-)}(\varepsilon_{\mathrm{R}\boldsymbol{k}\sigma})\,\mathrm{e}^{-\mathrm{i}(\varepsilon_{\mathrm{R}\boldsymbol{k}\sigma}+L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu'}\right]\rho_{\mathrm{QS}}^{(n_\mathrm{L},n_\mathrm{R}-1)}(t)\,d_\mu^\dagger.
\end{aligned}
\tag{3.23}
$$

若电极的态密度选择洛伦兹截断, 即

$$
\rho_{\alpha\sigma}(\varepsilon)=\rho_{\alpha\sigma}g_\alpha(\varepsilon)=\rho_{\alpha\sigma}\frac{W^2}{(\varepsilon-\mu_\alpha)^2+W^2},
\tag{3.24}
$$

并定义如下超算符和隧穿概率 $\Gamma_{\alpha\sigma}^{\mu\mu'}$:

$$
A_{\alpha\mu'}^{(\pm)}(t)=\frac{1}{\hbar}\int\mathrm{d}\varepsilon\int_{t_0}^{t}\mathrm{d}t_1 g_\alpha(\varepsilon)\,f_\alpha^{(\pm)}(\varepsilon)\,\mathrm{e}^{-\mathrm{i}(\varepsilon+L_{\mathrm{QS}})(t-t_1)/\hbar}d_{\mu'},
\tag{3.25}
$$

$$
\Gamma_{\alpha\sigma}^{\mu\mu'}=\sum_{\alpha\mu\mu'\sigma}\frac{2\pi\rho_{\alpha\sigma}\left|t_{\alpha\sigma}^{\mu\mu'}\right|^2}{\hbar},
\tag{3.26}
$$

则式 (3.1) 可以表示为

$$
\begin{aligned}
&\frac{\mathrm{d}\rho_{\mathrm{QS}}^{(n_\mathrm{L},n_\mathrm{R})}(t)}{\mathrm{d}t}\\
&=-\frac{\mathrm{i}}{\hbar}\left[H_{\mathrm{QS}},\rho_{\mathrm{QS}}^{(n_\mathrm{L},n_\mathrm{R})}(t)\right]-\sum_{\alpha\mu\mu'\sigma}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2\pi}\left[d_\mu^\dagger A_{\alpha\mu'}^{(-)}(t)\,\rho_{\mathrm{QS}}^{(n_\mathrm{L},n_\mathrm{R})}(t)\right.
\end{aligned}
$$

$$
+\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\,A_{\alpha\mu'}^{(+)}(t)\,d_{\mu}^{\dagger}-d_{\mu}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,A_{\mathrm{L}\mu'}^{(+)}(t)-d_{\mu}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,A_{\mathrm{R}\mu'}^{(+)}(t)
$$

$$
-A_{\mathrm{L}\mu'}^{(-)}(t)\,\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{\mu}^{\dagger}-A_{\mathrm{R}\mu'}^{(-)}(t)\,\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{\mu}^{\dagger}+\mathrm{H.c.}\Big], \tag{3.27}
$$

若只记录电子从所研究量子系统隧穿到漏极的电子数 $n$, 则上式可简化为 [2]

$$
\begin{aligned}
&\frac{\mathrm{d}\rho_{\mathrm{QS}}^{(n)}(t)}{\mathrm{d}t}\\
&=-\frac{\mathrm{i}}{\hbar}\left[H_{\mathrm{QS}},\rho_{\mathrm{QS}}^{(n)}(t)\right]-\sum_{\alpha\mu\mu'\boldsymbol{\sigma}}\frac{\Gamma_{\alpha\sigma}^{\mu\mu'}}{2\pi}\Big[d_{\mu}^{\dagger}A_{\alpha\mu'}^{(-)}(t)\,\rho_{\mathrm{QS}}^{(n)}(t)\\
&\quad+\rho_{\mathrm{QS}}^{(n)}(t)\,A_{\alpha\mu'}^{(+)}(t)\,d_{\mu}^{\dagger}-d_{\mu}^{\dagger}\rho_{\mathrm{QS}}^{(n)}(t)\,A_{\mathrm{L}\mu'}^{(+)}(t)-d_{\mu}^{\dagger}\rho_{\mathrm{QS}}^{(n+1)}(t)\,A_{\mathrm{R}\mu'}^{(+)}(t)\\
&\quad-A_{\mathrm{L}\mu'}^{(-)}(t)\,\rho_{\mathrm{QS}}^{(n)}(t)\,d_{\mu}^{\dagger}-A_{\mathrm{R}\mu'}^{(-)}(t)\,\rho_{\mathrm{QS}}^{(n-1)}(t)\,d_{\mu}^{\dagger}+\mathrm{H.c.}\Big],
\end{aligned}\tag{3.28}
$$

式 (3.28) 即时间局域的粒子数分辨量子主方程, 它是计算高阶电流累积矩的起点.

## 3.2　电子计数统计理论

在量子输运问题中, 电子的全计数统计可以提供到 $t$ 时刻为止有 $n$ 个电子隧穿过所研究量子系统到达漏极 (右电极) 的概率分布 $P(n,t)$ 的所有信息. 但是, 在实际计算中并不直接从粒子数分辨的量子主方程求解概率分布 $P(n,t)$, 而是采用累积矩生成函数的方法. 在数学上, 累积矩生成函数定义为 [3,4]

$$
\mathrm{e}^{-F(\chi)}=\sum_{n}P(n,t)\,\mathrm{e}^{\mathrm{i}n\chi}, \tag{3.29}
$$

其中, $\chi$ 为计数场. 所有的零频电流累积矩都可以通过对累积矩生成函数求关于 $\chi$ 的微分得到

$$
C_k=-\left(-\mathrm{i}\frac{\partial}{\partial\chi}\right)^{k}F(\chi)\bigg|_{\chi\to0}. \tag{3.30}
$$

在长时间极限下, 前四阶累积矩直接联系到开放量子系统的电子输运特性. 例如, 一阶累积矩 (传输电子数目分布的峰值位置) 给出了平均电流:

$$
\langle I\rangle=C_1/t, \tag{3.31}
$$

散粒噪声联系到二阶累积矩 (传输电子数目分布的峰宽):

$$
S(0)=2\mathrm{e}^2\left(\overline{n^2}-\bar{n}^2\right)\Big/t=2\mathrm{e}^2C_2/t, \tag{3.32}
$$

三阶和四阶累积矩:

$$
C_3=\overline{(n-\bar{n})^3}, \tag{3.33}
$$

$$C_4 = \overline{(n-\bar{n})^4} - 3\overline{(n-\bar{n})^2}^2, \tag{3.34}$$

分别刻画了传输电子数目分布的偏斜度和峭度. 这里, $\overline{(\cdots)} = \sum\limits_n (\cdots) P(n,t)$. 此外, 散粒噪声、偏斜度和峭度通常用 Fano 因子 $F_2 = C_2/C_1$、$F_3 = C_3/C_1$ 和 $F_4 = C_4/C_1$ 分别表示.

## 3.3 电流高阶累积矩的计算方法：适合解析计算

为了计算电流的前四阶电流累积矩, 首先计算其累积矩生成函数, 为此定义

$$S(\chi,t) = \sum_n \rho^{(n)}(t)\,\mathrm{e}^{\mathrm{i}n\chi}, \tag{3.35}$$

由式 (3.29) 可知

$$\mathrm{e}^{-F(\chi)} = \mathrm{tr}\left[S(\chi,t)\right]. \tag{3.36}$$

由于式 (3.28) 有如下形式：

$$\dot{\rho}^{(n)} = A_0\rho^{(n)} + C_{+1}\rho^{(n+1)} + D_{-1}\rho^{(n-1)}, \tag{3.37}$$

因而 $S(\chi,t)$ 满足：

$$\dot{S} = A_0 S + \mathrm{e}^{-\mathrm{i}\chi}C_{+1}S + \mathrm{e}^{\mathrm{i}\chi}D_{-1}S \equiv L(\chi)\,S. \tag{3.38}$$

其中, $S$ 是列矩阵, $A_0$, $C_{+1}$, $D_{-1}$ 为三个方矩阵; $L(\chi)$ 的具体形式可以通过对式 (3.37) 的矩阵元作分离傅里叶变换得到. 在低频极限下, 计数时间 (即测量时间) 远大于电子通过开放量子系统的隧穿时间. 此时, $F(\chi)$ 有如下的形式 [4-9]：

$$F(\chi) = -\lambda_0(\chi)\,t, \tag{3.39}$$

其中, $\lambda_0(\chi)$ 是 $L(\chi)$ 的本征值, 且满足当 $\chi \to 0$ 时, 其数值趋于零. 根据累积矩的定义, 可将 $\lambda_0(\chi)$ 写成如下形式：

$$\lambda_0(\chi) = \sum_{k=1}^{\infty} \frac{C_k}{t}\frac{(\mathrm{i}\chi)^k}{k!}. \tag{3.40}$$

将式 (3.40) 代入 $|L(\chi) - \lambda_1(\chi)\,I| = 0$, 并将其行列式按 $(\mathrm{i}\chi)^k$ 展开, 考虑到 $\mathrm{i}\chi$ 是任意的, 因而, 可以通过令 $(\mathrm{i}\chi)^k$ 的系数等于零来依次计算 $C_k/t$.

## 3.4 电流高阶累积矩的计算方法：适合数值计算

当矩阵 $L(\chi)$ 的维数较大时, 3.3 节给出的基于符号运算计算开放量子系统前四阶累积矩的方法, 由于其巨大的计算量而将不再适用. 在本节中, 给出一种基于瑞利–薛定谔 (Rayleigh-Schrödinger) 微扰理论 [10] 的完全数值化的计算开放量子系统前四阶累积矩的方法 [6-9,11]. 首先, 将矩阵 $L(\chi)$ 按 $\chi$ 的幂次展开到四阶

$$L(\chi) = L_0 + L_1(\mathrm{i}\chi) + \frac{1}{2!}L_2(\mathrm{i}\chi)^2 + \frac{1}{3!}L_3(\mathrm{i}\chi)^3 + \frac{1}{4!}L_4(\mathrm{i}\chi)^4 + \cdots, \tag{3.41}$$

其次, 引入如下两个超算符：

$$\tilde{P} = |0\rangle\rangle\langle\langle\tilde{0}|, \tag{3.42}$$

$$\tilde{Q} = 1 - \tilde{P}, \tag{3.43}$$

它们分别满足如下关系：

$$\tilde{P}L_0 = L_0\tilde{P} = 0, \tag{3.44}$$

$$\tilde{Q}L_0 = L_0\tilde{Q} = L_0, \tag{3.45}$$

其中, $|0\rangle\rangle$ 是矩阵 $L_0$ 右矢的稳态 $\rho^{\mathrm{stat}}$, 满足 $L_0|0\rangle\rangle = 0$; 而 $\langle\langle\tilde{0}|$ 是其相应的左矢, 满足 $\langle\langle\tilde{0}|L_0 = 0$, 它们的内积为 $\langle\langle\tilde{0}|0\rangle\rangle = 1$. 鉴于 $L_0$ 的奇异性, 继续引入 $L_0$ 的赝逆算符：

$$\tilde{R} = \tilde{Q}(L_0)^{-1}\tilde{Q}, \tag{3.46}$$

其中, 算符 $\tilde{R}$ 定义在算符 $\tilde{Q}$ 张开的子空间, 因而其逆是存在的. 根据瑞利–薛定谔微扰理论, 可得开放量子系统的前四阶累积矩分别为

$$C_1/t = \langle\langle\tilde{0}|L_1|0\rangle\rangle, \tag{3.47}$$

$$C_2/t = \langle\langle\tilde{0}|L_2|0\rangle\rangle - 2\langle\langle\tilde{0}|L_1\tilde{R}L_1|0\rangle\rangle, \tag{3.48}$$

$$\begin{aligned}
C_3/t = {} & \langle\langle\tilde{0}|L_3|0\rangle\rangle - 3\left[\langle\langle\tilde{0}|L_1\tilde{R}L_2|0\rangle\rangle + \langle\langle\tilde{0}|L_2\tilde{R}L_1|0\rangle\rangle\right] \\
& - 6\left[\langle\langle\tilde{0}|L_1\tilde{R}\tilde{R}L_1|0\rangle\rangle\langle\langle\tilde{0}|L_1|0\rangle\rangle - \langle\langle\tilde{0}|L_1\tilde{R}L_1\tilde{R}L_1|0\rangle\rangle\right] \\
= {} & \langle\langle\tilde{0}|L_3|0\rangle\rangle - 3\langle\langle\tilde{0}|\left(L_1\tilde{R}L_2 + L_2\tilde{R}L_1\right)|0\rangle\rangle \\
& - 6\langle\langle\tilde{0}|L_1\tilde{R}\left(\tilde{R}L_1\tilde{P} - L_1\tilde{R}\right)L_1|0\rangle\rangle,
\end{aligned} \tag{3.49}$$

$$C_4/t = \langle\langle\tilde{0}|L_4|0\rangle\rangle - 6\langle\langle\tilde{0}|L_2\tilde{R}L_2|0\rangle\rangle$$

$$
\begin{aligned}
&- 4\left\langle\left\langle\tilde{0}\right|\left(L_1\tilde{R}L_3+L_3\tilde{R}L_1\right)\left|0\right\rangle\right\rangle - 12\left\langle\left\langle\tilde{0}\right|L_1\tilde{R}\left(\tilde{R}L_2\tilde{P}-L_2\tilde{R}\right)L_1\left|0\right\rangle\right\rangle\\
&- 12\left\langle\left\langle\tilde{0}\right|L_1\tilde{R}\left(\tilde{R}L_1\tilde{P}-L_1\tilde{R}\right)L_2\left|0\right\rangle\right\rangle - 12\left\langle\left\langle\tilde{0}\right|L_2\tilde{R}\left(\tilde{R}L_1\tilde{P}-L_1\tilde{R}\right)L_1\left|0\right\rangle\right\rangle\\
&- 24\left\langle\left\langle\tilde{0}\right|L_1\tilde{R}\left(\tilde{R}\tilde{R}L_1\tilde{P}L_1\tilde{P}-\tilde{R}L_1\tilde{P}L_1\tilde{R}-L_1\tilde{R}\tilde{R}L_1\tilde{P}\right.\right.\\
&\left.\left.-\ \tilde{R}L_1\tilde{R}L_1\tilde{P}+L_1\tilde{R}L_1\tilde{R}\right)L_1\left|0\right\rangle\right\rangle. \qquad (3.50)
\end{aligned}
$$

上面四式即为数值化计算开放量子系统前四阶累积矩的基础, 详细计算过程可见附录 F.

## 3.5 应用举例：单量子点模型

在本节中, 以与两个金属电极弱耦合的单能级量子点模型说明 3.3 和 3.4 两节中的计算方法. 此系统的哈密顿量可以描述为

$$
\begin{aligned}
H &= H_{\mathrm{dot}} + H_{\mathrm{leads}} + H_{\mathrm{T}}\\
&= \varepsilon_d a^\dagger a + \sum_{\alpha=\mathrm{L,R}}\sum_{\boldsymbol{k}}\varepsilon_{\alpha\boldsymbol{k}}d^\dagger_{\alpha\boldsymbol{k}}d_{\alpha\boldsymbol{k}} + \sum_{\alpha=\mathrm{L,R}}\sum_{\boldsymbol{k}}\left(t_{\alpha\boldsymbol{k}}a^\dagger d_{\alpha\boldsymbol{k}} + \mathrm{H.c.}\right), \qquad (3.51)
\end{aligned}
$$

其中, 第一、二项分别为单能级量子点和两个金属电极的哈密顿量, 第三项是电子在单量子点和金属电极之间的隧穿耦合. 若式 (2.17) 描述的微扰项缓慢打开, 为了保持 $t$ 为有限值, 选取 $\eta \to 0^+$, 此时 $t_0 \to -\infty$, 因此式 (3.25) 定义的超算符和式 (3.26) 定义的隧穿概率可以表示为

$$
\begin{aligned}
A_\alpha^{(\pm)}(t) &= \lim_{\eta\to0}\frac{1}{\hbar}\int \mathrm{d}\varepsilon g_\alpha(\varepsilon) f_\alpha^{(\pm)}(\varepsilon)\int_{-\infty}^{t}\mathrm{d}t_1 \mathrm{e}^{-\mathrm{i}(\varepsilon+L_{\mathrm{QD}})(t-t_1)/\hbar}\mathrm{e}^{\eta(t+t_1)}a\\
&= \lim_{\eta\to0}\int \mathrm{d}\varepsilon g_\alpha(\varepsilon) f_\alpha^{(\pm)}(\varepsilon)\frac{\mathrm{e}^{-\mathrm{i}(\varepsilon+L_{\mathrm{QD}}+\mathrm{i}\eta\hbar)t/\hbar}\mathrm{e}^{\mathrm{i}(\varepsilon+L_{\mathrm{QD}}-\mathrm{i}\eta\hbar)t/\hbar}}{\mathrm{i}\left(\varepsilon+L_{\mathrm{QS}}-\mathrm{i}\eta\hbar\right)}a\\
&= \lim_{\eta\to0}\int \mathrm{d}\varepsilon g_\alpha(\varepsilon) f_\alpha^{(\pm)}(\varepsilon)\frac{-\mathrm{i}\mathrm{e}^{2\eta t}\left(\varepsilon+L_{\mathrm{QD}}\right)+\mathrm{e}^{2\eta t}\eta\hbar}{\left(\varepsilon+L_{\mathrm{QD}}\right)^2+(\eta\hbar)^2}a\\
&= -\mathrm{iP}\int \mathrm{d}\varepsilon\frac{g_\alpha(\varepsilon) f_\alpha^{(\pm)}(\varepsilon)}{\varepsilon+L_{\mathrm{QS}}}a + \pi g_\alpha\left(-L_{\mathrm{QS}}\right) f_\alpha^{(\pm)}\left(-L_{\mathrm{QS}}\right)a, \qquad (3.52)
\end{aligned}
$$

$$
\Gamma_\alpha = \frac{2\pi\rho_\alpha\left|t_\alpha\right|^2}{\hbar}. \qquad (3.53)
$$

若选择空占据态 $|0\rangle$ 和占据态 $|1\rangle$ 作为基矢将量子点的哈密顿量对角化, 相应的能量本征值和本征态为

$$\begin{cases} H_{\mathrm{dot}}\left|0\right\rangle = 0, & \varepsilon_0 = 0 \\ H_{\mathrm{dot}}\left|1\right\rangle = \varepsilon_1\left|1\right\rangle, & \varepsilon_1 = \varepsilon_d \end{cases}. \tag{3.54}$$

尤其是在此基矢组下, 量子点的密度矩阵仅有对角元, 此时式 (3.52) 右边的第一项将与其共轭项相互抵消, 因此, 在宽带近似下其粒子数分辨量子主方程可以简化为

$$\begin{aligned} &\frac{\mathrm{d}\rho_{\mathrm{QD}}^{(n)}(t)}{\mathrm{d}t} \\ =& -\Gamma_{\mathrm{L}}a^{\dagger}A_{\mathrm{L}}^{(-)}(t)\,\rho_{\mathrm{QD}}^{(n)}(t) - \Gamma_{\mathrm{R}}a^{\dagger}A_{\mathrm{R}}^{(-)}(t)\,\rho_{\mathrm{QD}}^{(n)}(t) - \Gamma_{\mathrm{L}}\rho_{\mathrm{QD}}^{(n)}(t)\,A_{\mathrm{L}}^{(+)}(t)\,a^{\dagger} \\ & - \Gamma_{\mathrm{R}}\rho_{\mathrm{QD}}^{(n)}(t)\,A_{\mathrm{R}}^{(+)}(t)\,a^{\dagger} + \Gamma_{\mathrm{L}}a^{\dagger}\rho_{\mathrm{QD}}^{(n)}(t)\,A_{\mathrm{L}}^{(+)}(t) + \Gamma_{\mathrm{R}}a^{\dagger}\rho_{\mathrm{QD}}^{(n+1)}(t)\,A_{\mathrm{R}}^{(+)}(t) \\ & + \Gamma_{\mathrm{L}}A_{\mathrm{L}}^{(-)}(t)\,\rho_{\mathrm{QD}}^{(n)}(t)\,a^{\dagger} + \Gamma_{\mathrm{R}}A_{\mathrm{R}}^{(-)}(t)\,\rho_{\mathrm{QD}}^{(n-1)}(t)\,a^{\dagger}, \end{aligned} \tag{3.55}$$

其中

$$A_{\alpha}^{(\pm)}(t) = f_{\alpha}^{(\pm)}(-L_{\mathrm{QD}})\,a = f_{\alpha}^{(\pm)}(\varepsilon_d), \tag{3.56}$$

在式 (3.56) 的计算中使用了 $L_{\mathrm{QD}}^{n}a = (-\varepsilon_0)^n\,a$. 为方便计算, 考虑零温极限和大偏压情形 ($\mu_{\mathrm{L}} \gg \varepsilon_0 \gg \mu_{\mathrm{R}}$), 此时, 式 (3.56) 可以简化为

$$\begin{cases} A_{\mathrm{L}}^{(+)} = \Gamma_{\mathrm{L}}a, & A_{\mathrm{L}}^{(-)} = 0 \\ A_{\mathrm{R}}^{(+)} = 0, & A_{\mathrm{R}}^{(-)} = \Gamma_{\mathrm{R}}a \end{cases}. \tag{3.57}$$

相应地式 (3.55) 可以简化为

$$\frac{\mathrm{d}\rho_{\mathrm{QD}}^{(n)}(t)}{\mathrm{d}t} = -\Gamma_{\mathrm{R}}a^{\dagger}a\rho_{\mathrm{QD}}^{(n)}(t) - \Gamma_{\mathrm{L}}\rho_{\mathrm{QD}}^{(n)}(t)\,aa^{\dagger} + \Gamma_{\mathrm{L}}a^{\dagger}\rho_{\mathrm{QD}}^{(n)}(t)\,a + \Gamma_{\mathrm{R}}a\rho_{\mathrm{QD}}^{(n-1)}(t)\,a^{\dagger}, \tag{3.58}$$

将空占据态 $\left|0\right\rangle$ 和占据态 $\left|1\right\rangle$ 分别作用到式 (3.58) 两边, 可得

$$\begin{cases} \dot{\rho}_{00}^{(n)} = -\Gamma_{\mathrm{L}}\rho_{00}^{(n)} + \Gamma_{\mathrm{R}}\rho_{11}^{(n-1)} \\ \dot{\rho}_{11}^{(n)} = \Gamma_{\mathrm{L}}\rho_{00}^{(n)} - \Gamma_{\mathrm{R}}\rho_{11}^{(n)} \end{cases}, \tag{3.59}$$

其中 $\rho_{00}^{(n)} = \left\langle 0\right|\rho^{(n)}\left|0\right\rangle$ 和 $\rho_{11}^{(n)} = \left\langle 1\right|\rho^{(n)}\left|1\right\rangle$. 对式 (3.59) 做分离傅里叶变换 $\sum\limits_{n}\mathrm{e}^{\mathrm{i}n\chi}$ 可得

$$L(\chi) = \begin{pmatrix} -\Gamma_{\mathrm{L}} & \Gamma_{\mathrm{R}}\mathrm{e}^{\mathrm{i}\chi} \\ \Gamma_{\mathrm{L}} & -\Gamma_{\mathrm{R}} \end{pmatrix}. \tag{3.60}$$

下面, 用 3.3 节的方法计算单能级量子点的前三阶电流累积矩. 将式 (3.60) 和式 (3.40) 代入 $\left|L(\chi) - \lambda_1(\chi)\,I\right| = 0$, 可得

$$\begin{vmatrix} -\Gamma_{\mathrm{L}}-\mathrm{i}\frac{C_1}{t}\chi+\frac{1}{2}\frac{C_2}{t}\chi^2+\mathrm{i}\frac{C_3}{t}\frac{\chi^3}{6} & \Gamma_{\mathrm{R}}\left(1+\mathrm{i}\chi-\frac{1}{2}\chi^2-\mathrm{i}\frac{\chi^3}{6}\right) \\ \Gamma_{\mathrm{L}} & -\Gamma_{\mathrm{R}}-\mathrm{i}\frac{C_1}{t}\chi+\frac{1}{2}\frac{C_2}{t}\chi^2+\mathrm{i}\frac{C_3}{t}\frac{\chi^3}{6} \end{vmatrix}=0, \quad (3.61)$$

将上式左边按 $\chi$ 的幂级数 $\chi^k$ 展开可得

$$\begin{aligned} |L_\chi-\lambda_1(\chi)I| = & \left(\Gamma_{\mathrm{L}}\frac{C_1}{t}+\Gamma_{\mathrm{R}}\frac{C_1}{t}-\Gamma_{\mathrm{L}}\Gamma_{\mathrm{R}}\right)(\mathrm{i}\chi) \\ & +\left[\frac{\Gamma_{\mathrm{L}}}{2}\frac{C_2}{t}+\left(\frac{C_1}{t}\right)^2+\frac{\Gamma_{\mathrm{R}}}{2}\frac{C_2}{t}-\frac{1}{2}\Gamma_{\mathrm{L}}\Gamma_{\mathrm{R}}\right](\mathrm{i}\chi)^2 \\ & +\left(\frac{\Gamma_{\mathrm{L}}}{6}\frac{C_3}{t}+\frac{C_2}{t}\frac{C_1}{t}+\frac{\Gamma_{\mathrm{R}}}{6}\frac{C_3}{t}-\frac{\Gamma_{\mathrm{L}}\Gamma_{\mathrm{R}}}{6}\right)(\mathrm{i}\chi)^3+\cdots, \end{aligned} \quad (3.62)$$

由于式 (3.62) 行列式的值为零, 且 $\mathrm{i}\chi$ 是任意的, 因而, 可以得到如下的联立方程组:

$$\begin{cases} \Gamma_{\mathrm{L}}\frac{C_1}{t}+\Gamma_{\mathrm{R}}\frac{C_1}{t}-\Gamma_{\mathrm{L}}\Gamma_{\mathrm{R}}=0 \\ \frac{\Gamma_{\mathrm{L}}}{2}\frac{C_2}{t}+\left(\frac{C_1}{t}\right)^2+\frac{\Gamma_{\mathrm{R}}}{2}\frac{C_2}{t}-\frac{1}{2}\Gamma_{\mathrm{L}}\Gamma_{\mathrm{R}}=0 \\ \frac{\Gamma_{\mathrm{L}}}{6}\frac{C_3}{t}+\frac{C_2}{t}\frac{C_1}{t}+\frac{\Gamma_{\mathrm{R}}}{6}\frac{C_3}{t}-\frac{\Gamma_{\mathrm{L}}\Gamma_{\mathrm{R}}}{6}=0 \end{cases}, \quad (3.63)$$

通过依次求解方程组 (3.63), 可以得到前三阶电流累积矩为

$$\begin{cases} \frac{C_1}{t}=\frac{\Gamma_{\mathrm{L}}\Gamma_{\mathrm{R}}}{\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}}} \\ \frac{C_2}{t}=\frac{\Gamma_{\mathrm{L}}^2+\Gamma_{\mathrm{R}}^2}{(\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}})^2}\frac{\Gamma_{\mathrm{L}}\Gamma_{\mathrm{R}}}{\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}}} \\ \frac{C_3}{t}=\frac{\Gamma_{\mathrm{R}}^4-2\Gamma_{\mathrm{R}}^3\Gamma_{\mathrm{L}}+6\Gamma_{\mathrm{R}}^2\Gamma_{\mathrm{L}}^2-2\Gamma_{\mathrm{R}}\Gamma_{\mathrm{L}}^3+\Gamma_{\mathrm{L}}^4}{(\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}})^4}\frac{\Gamma_{\mathrm{L}}\Gamma_{\mathrm{R}}}{\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}}} \end{cases}. \quad (3.64)$$

现在, 使用 3.4 节的方法处理上面同样的问题. 利用式 (3.60), 可以将矩阵 $L(\chi)$ 按 $\chi$ 的幂次展开为

$$\begin{aligned} L(\chi)= & \begin{pmatrix} -\Gamma_{\mathrm{L}} & \Gamma_{\mathrm{R}} \\ \Gamma_{\mathrm{L}} & -\Gamma_{\mathrm{R}} \end{pmatrix}+\begin{pmatrix} 0 & \mathrm{i}\Gamma_{\mathrm{R}} \\ 0 & 0 \end{pmatrix}\chi+\frac{1}{2!}\begin{pmatrix} 0 & -\Gamma_{\mathrm{R}} \\ 0 & 0 \end{pmatrix}\chi^2 \\ & +\frac{1}{3!}\begin{pmatrix} 0 & -\mathrm{i}\Gamma_{\mathrm{R}} \\ 0 & 0 \end{pmatrix}\chi^3+\cdots, \end{aligned} \quad (3.65)$$

因而, 有

$$L_0=\begin{pmatrix} -\Gamma_{\mathrm{L}} & \Gamma_{\mathrm{R}} \\ \Gamma_{\mathrm{L}} & -\Gamma_{\mathrm{R}} \end{pmatrix},\quad L_1=\begin{pmatrix} 0 & \mathrm{i}\Gamma_{\mathrm{R}} \\ 0 & 0 \end{pmatrix},$$
$$L_2=\begin{pmatrix} 0 & -\Gamma_{\mathrm{R}} \\ 0 & 0 \end{pmatrix},\quad L_3=\begin{pmatrix} 0 & -\mathrm{i}\Gamma_{\mathrm{R}} \\ 0 & 0 \end{pmatrix}. \tag{3.66}$$

利用矩阵 $L_0$, 很容易求出

$$|0\rangle\rangle=\frac{1}{\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}}}\begin{pmatrix} \Gamma_{\mathrm{R}} \\ \Gamma_{\mathrm{L}} \end{pmatrix},\quad \langle\langle\tilde{0}|=\begin{pmatrix} 1 & 1 \end{pmatrix}, \tag{3.67}$$

然后, 根据超算符 $\tilde{P}$ 和 $\tilde{Q}$ 的定义, 可以得到其具体形式为

$$\tilde{P}=\frac{1}{\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}}}\begin{pmatrix} \Gamma_{\mathrm{R}} & \Gamma_{\mathrm{R}} \\ \Gamma_{\mathrm{L}} & \Gamma_{\mathrm{L}} \end{pmatrix},\quad \tilde{Q}=\frac{1}{\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}}}\begin{pmatrix} \Gamma_{\mathrm{L}} & -\Gamma_{\mathrm{R}} \\ -\Gamma_{\mathrm{L}} & \Gamma_{\mathrm{R}} \end{pmatrix}. \tag{3.68}$$

此外, 根据赝逆算符 $R$ 的定义, 还需要知道矩阵 $L_0$ 的非零本征值和本征矢. 根据矩阵 $L_0$ 的形式, 可以求得

$$\lambda_\nu=-\left(\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}}\right),\quad |\nu\rangle\rangle=\begin{pmatrix} 1 \\ -1 \end{pmatrix},\quad \langle\langle\tilde{\nu}|=\frac{1}{\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}}}\begin{pmatrix} \Gamma_{\mathrm{L}} & -\Gamma_{\mathrm{R}} \end{pmatrix}, \tag{3.69}$$

因而, 赝逆算符 $\tilde{R}$ 的形式可以表示为

$$\tilde{R}=\tilde{Q}\left(L_0\right)^{-1}\tilde{Q}=\frac{1}{\lambda_\nu}\,|\nu\rangle\rangle\,\langle\langle\tilde{\nu}|=\frac{1}{\lambda_\nu}\tilde{Q}=-\frac{1}{\left(\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}}\right)^2}\begin{pmatrix} \Gamma_{\mathrm{L}} & -\Gamma_{\mathrm{R}} \\ -\Gamma_{\mathrm{L}} & \Gamma_{\mathrm{R}} \end{pmatrix}. \tag{3.70}$$

根据前三阶累积矩的表达式 (3.47) ∼ 式 (3.49), 并利用式 (3.66)、式 (3.68) 和式 (3.70), 可以直接计算其前三阶电流累积矩. 对于前两阶的累积矩, 其表达式分别为

$$\begin{aligned} C_1/t&=\langle\langle\tilde{0}|\,L_1\,|0\rangle\rangle\,/\mathrm{i}\\ &=\frac{-\mathrm{i}}{\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}}}\begin{pmatrix} 1 & 1 \end{pmatrix}\begin{pmatrix} 0 & \mathrm{i}\Gamma_{\mathrm{R}} \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \Gamma_{\mathrm{R}} \\ \Gamma_{\mathrm{L}} \end{pmatrix}\\ &=\frac{-\mathrm{i}}{\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}}}\begin{pmatrix} 0 & \mathrm{i}\Gamma_{\mathrm{R}} \end{pmatrix}\begin{pmatrix} \Gamma_{\mathrm{R}} \\ \Gamma_{\mathrm{L}} \end{pmatrix}=\frac{-\mathrm{i}}{\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}}}\left(\mathrm{i}\Gamma_{\mathrm{R}}\Gamma_{\mathrm{L}}\right)=\frac{\Gamma_{\mathrm{L}}\Gamma_{\mathrm{R}}}{\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}}}, \end{aligned} \tag{3.71}$$

$$\begin{aligned} C_2/t&=\left[\langle\langle\tilde{0}|\,L_2\,|0\rangle\rangle-2\,\langle\langle\tilde{0}|\,L_1\tilde{R}L_1\,|0\rangle\rangle\right]/\mathrm{i}^2\\ &=-\frac{1}{\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}}}\begin{pmatrix} 1 & 1 \end{pmatrix}\begin{pmatrix} 0 & -\Gamma_{\mathrm{R}} \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \Gamma_{\mathrm{R}} \\ \Gamma_{\mathrm{L}} \end{pmatrix} \end{aligned}$$

$$
\begin{aligned}
&-\frac{2}{(\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}})^3}\begin{pmatrix} 1 & 1 \end{pmatrix}\begin{pmatrix} 0 & \mathrm{i}\Gamma_{\mathrm{R}} \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \Gamma_{\mathrm{L}} & -\Gamma_{\mathrm{R}} \\ -\Gamma_{\mathrm{L}} & \Gamma_{\mathrm{R}} \end{pmatrix}\begin{pmatrix} 0 & \mathrm{i}\Gamma_{\mathrm{R}} \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \Gamma_{\mathrm{R}} \\ \Gamma_{\mathrm{L}} \end{pmatrix}\\
=&-\frac{1}{\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}}}\begin{pmatrix} 0 & -\Gamma_{\mathrm{R}} \end{pmatrix}\begin{pmatrix} \Gamma_{\mathrm{R}} \\ \Gamma_{\mathrm{L}} \end{pmatrix}\\
&-\frac{2}{(\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}})^3}\begin{pmatrix} 0 & \mathrm{i}\Gamma_{\mathrm{R}} \end{pmatrix}\begin{pmatrix} \Gamma_{\mathrm{L}} & -\Gamma_{\mathrm{R}} \\ -\Gamma_{\mathrm{L}} & \Gamma_{\mathrm{R}} \end{pmatrix}\begin{pmatrix} \mathrm{i}\Gamma_{\mathrm{L}}\Gamma_{\mathrm{R}} \\ 0 \end{pmatrix}\\
=&\frac{\Gamma_{\mathrm{L}}\Gamma_{\mathrm{R}}}{\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}}}-\frac{2}{(\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}})^3}\begin{pmatrix} -\mathrm{i}\Gamma_{\mathrm{L}}\Gamma_{\mathrm{R}} & \mathrm{i}\Gamma_{\mathrm{R}}\Gamma_{\mathrm{R}} \end{pmatrix}\begin{pmatrix} \mathrm{i}\Gamma_{\mathrm{L}}\Gamma_{\mathrm{R}} \\ 0 \end{pmatrix}\\
=&\frac{\Gamma_{\mathrm{L}}\Gamma_{\mathrm{R}}}{\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}}}-\frac{2\Gamma_{\mathrm{L}}^2\Gamma_{\mathrm{R}}^2}{(\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}})^3}=\frac{\Gamma_{\mathrm{L}}\Gamma_{\mathrm{R}}}{\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}}}\frac{\Gamma_{\mathrm{L}}^2+\Gamma_{\mathrm{R}}^2}{(\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}})^2}.
\end{aligned}\tag{3.72}
$$

同样, 可以求出第三阶的累积矩, 其表达式与式 (3.64) 相同 [12,13]. 需要指出的是, 在实际计算中, 具体选取何种方法依赖于开放量子系统约化密度矩阵的维数大小.

## 参 考 文 献


[1] Li X Q, Luo J Y, Yang Y G, et al. Quantum master-equation approach to quantum transport through mesoscopic systems. Phys. Rev. B, 2005, 71: 205304.

[2] Xue H B, Jiao H J, Liang J Q, et al. Non-Markovian full counting statistics in quantum dot molecules. Sci. Rep., 2015, 5: 8978.

[3] Wang S K, Jiao H J, Li F, et al. Full counting statistics of transport through two-channel Coulomb blockade systems. Phys. Rev. B, 2007, 76: 125416.

[4] Bagrets D A, Nazarov Y V. Full counting statistics of charge transfer in Coulomb blockade systems. Phys. Rev. B, 2003, 67: 085316.

[5] Kießlich G, Samuelsson P, Wacker A, et al. Counting statistics and decoherence in coupled quantum dots. Phys. Rev. B, 2006, 73: 033312.

[6] Flindt C, Novotný T, Braggio A, et al. Counting statistics of non-Markovian quantum stochastic processes. Phys. Rev. Lett., 2008, 100: 150601.

[7] Flindt C, Novotný T, Braggio A, et al. Counting statistics of transport through Coulomb blockade nanostructures: High-order cumulants and non-Markovian effects. Phys. Rev. B, 2010, 82: 155407.

[8] Flindt C, Novotný T, Jauho A P. Full counting statistics of nano-electromechanical systems. EPL, 2005, 69: 475-481.

[9] Groth C W, Michaelis B, Beenakker C W J. Counting statistics of coherent population trapping in quantum dots. Phys. Rev. B, 2006, 74: 125315.

[10] Sakurai J J, Napolitano J J. Modern Quantum Mechanics. 2nd ed. Boston: Addison-Wesley, 1995: Chap. 5.

[11] Xue H B, Nie Y H, Li Z J, et al. Effects of magnetic field and transverse anisotropy on full counting statistics in single-molecule magnet. J. Appl. Phys., 2011, 109: 083706.

[12] de Jong M J M. Distribution of transmitted charge through a double-barrier junction. Phys. Rev. B, 1996, 54: 8144-8149.

[13] Jauho A P, Flindt C, Novotný T, et al. Current and current fluctuations in quantum shuttles. Phys. Fluids, 2005, 17: 100613.

# 第 4 章　四阶非马尔可夫的电子计数统计理论

在单分子结和微纳器件的量子输运中, 量子系统与源极、漏极的耦合强度通常处于中间耦合强度区域, 此时, 传导电子的隧穿过程除了顺序隧穿, 还有更高阶的共隧穿过程, 即所谓的共隧穿辅助的顺序隧穿过程. 在本章中, 首先, 给出时间局域的四阶量子主方程在相互作用绘景和薛定谔绘景中的具体表达式; 其次, 基于时间局域的四阶非马尔可夫量子主方程推导其对应的粒子数分辨量子主方程; 最后, 给出计算电流前四阶累积矩的计算方法.

## 4.1　四阶时间局域的量子主方程：相互作用绘景

在开放量子系统中, 在共隧穿极限下, 即同时考虑电子的顺序隧穿和共隧穿过程, 系统密度矩阵的运动方程可表示为

$$\frac{\partial}{\partial t}P\rho_{\mathrm{I}}(t)=K_2(t)\,P\rho_{\mathrm{I}}(t)+K_4(t)\,P\rho_{\mathrm{I}}(t),\tag{4.1}$$

其中, 式 (4.1) 中的第一项描述了电子的顺序隧穿过程 (已在第 3 章讨论), 第二项描述了电子的共隧穿过程. 由式 (2.152) 可知, 电子的共隧穿过程可表示为

$$\begin{aligned}&K_4(t)\,P\rho_{\mathrm{I}}(t)\\=&\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 PL_{\mathrm{I}}(t)\,L_{\mathrm{I}}(t_1)\,L_{\mathrm{I}}(t_2)\,L_{\mathrm{I}}(t_3)\,P\rho_{\mathrm{I}}(t)\\&-\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 PL_{\mathrm{I}}(t)\,L_{\mathrm{I}}(t_1)\,PL_{\mathrm{I}}(t_2)\,L_{\mathrm{I}}(t_3)\,P\rho_{\mathrm{I}}(t)\\&-\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 PL_{\mathrm{I}}(t)\,L_{\mathrm{I}}(t_2)\,PL_{\mathrm{I}}(t_1)\,L_{\mathrm{I}}(t_3)\,P\rho_{\mathrm{I}}(t)\\&-\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 PL_{\mathrm{I}}(t)\,L_{\mathrm{I}}(t_3)\,PL_{\mathrm{I}}(t_1)\,L_{\mathrm{I}}(t_2)\,P\rho_{\mathrm{I}}(t).\end{aligned}\tag{4.2}$$

根据超算符 $P$ 和 $L_{\mathrm{I}}$ 的定义, 将式 (4.2) 右边的第一项展开可得

$$\begin{aligned}&K_4(t)\,P\rho_{\mathrm{I}}(t)\big|_{01}\\=&\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\&\times\mathrm{tr}_{\mathrm{leads}}\left[H_{\mathrm{T,I}}(t),\left[H_{\mathrm{T,I}}(t_1),\left[H_{\mathrm{T,I}}(t_2),\left[H_{\mathrm{T,I}}(t_3),\rho_{\mathrm{QS,I}}(t)\otimes\rho_{\mathrm{leads}}\right]\right]\right]\right]\otimes\rho_{\mathrm{leads}},\end{aligned}\tag{4.3}$$

这里, 取 $\hbar \equiv 1$. 考虑到式 (4.1) 左边可表示为

$$\frac{\partial}{\partial t} P \rho_{\mathrm{I}}(t) = \frac{\partial \rho_{\mathrm{QS,I}}(t)}{\partial t} \otimes \rho_{\mathrm{leads}}, \tag{4.4}$$

因此, 式 (4.3) 可进一步表示为

$$\begin{aligned}
K_4(t) P\rho_{\mathrm{I}}(t)\big|_{01} = & \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \int_{t_0}^{t_2} \mathrm{d}t_3 \\
& \times \{\mathrm{tr}_{\mathrm{leads}}[H_{\mathrm{T,I}}(t) H_{\mathrm{T,I}}(t_1) H_{\mathrm{T,I}}(t_2) H_{\mathrm{T,I}}(t_3) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}}] \\
& - \mathrm{tr}_{\mathrm{leads}}[H_{\mathrm{T,I}}(t) H_{\mathrm{T,I}}(t_1) H_{\mathrm{T,I}}(t_2) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t_3)] \\
& - \mathrm{tr}_{\mathrm{leads}}[H_{\mathrm{T,I}}(t) H_{\mathrm{T,I}}(t_1) H_{\mathrm{T,I}}(t_3) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t_2)] \\
& + \mathrm{tr}_{\mathrm{leads}}[H_{\mathrm{T,I}}(t) H_{\mathrm{T,I}}(t_1) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t_3) H_{\mathrm{T,I}}(t_2)] \\
& - \mathrm{tr}_{\mathrm{leads}}[H_{\mathrm{T,I}}(t) H_{\mathrm{T,I}}(t_2) H_{\mathrm{T,I}}(t_3) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t_1)] \\
& + \mathrm{tr}_{\mathrm{leads}}[H_{\mathrm{T,I}}(t) H_{\mathrm{T,I}}(t_2) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t_3) H_{\mathrm{T,I}}(t_1)] \\
& + \mathrm{tr}_{\mathrm{leads}}[H_{\mathrm{T,I}}(t) H_{\mathrm{T,I}}(t_3) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t_2) H_{\mathrm{T,I}}(t_1)] \\
& - \mathrm{tr}_{\mathrm{leads}}[H_{\mathrm{T,I}}(t) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t_3) H_{\mathrm{T,I}}(t_2) H_{\mathrm{T,I}}(t_1)] \\
& - \mathrm{tr}_{\mathrm{leads}}[H_{\mathrm{T,I}}(t_1) H_{\mathrm{T,I}}(t_2) H_{\mathrm{T,I}}(t_3) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t)] \\
& + \mathrm{tr}_{\mathrm{leads}}[H_{\mathrm{T,I}}(t_1) H_{\mathrm{T,I}}(t_2) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t_3) H_{\mathrm{T,I}}(t)] \\
& + \mathrm{tr}_{\mathrm{leads}}[H_{\mathrm{T,I}}(t_1) H_{\mathrm{T,I}}(t_3) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t_2) H_{\mathrm{T,I}}(t)] \\
& - \mathrm{tr}_{\mathrm{leads}}[H_{\mathrm{T,I}}(t_1) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t_3) H_{\mathrm{T,I}}(t_2) H_{\mathrm{T,I}}(t)] \\
& + \mathrm{tr}_{\mathrm{leads}}[H_{\mathrm{T,I}}(t_2) H_{\mathrm{T,I}}(t_3) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t_1) H_{\mathrm{T,I}}(t)] \\
& - \mathrm{tr}_{\mathrm{leads}}[H_{\mathrm{T,I}}(t_2) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t_3) H_{\mathrm{T,I}}(t_1) H_{\mathrm{T,I}}(t)] \\
& - \mathrm{tr}_{\mathrm{leads}}[H_{\mathrm{T,I}}(t_3) \rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t_2) H_{\mathrm{T,I}}(t_1) H_{\mathrm{T,I}}(t)] \\
& + \mathrm{tr}_{\mathrm{leads}}[\rho_{\mathrm{QS,I}}(t) \otimes \rho_{\mathrm{leads}} H_{\mathrm{T,I}}(t_3) H_{\mathrm{T,I}}(t_2) H_{\mathrm{T,I}}(t_1) H_{\mathrm{T,I}}(t)]\},
\end{aligned} \tag{4.5}$$

为方便推导, 定义

$$F_\mu = \sum_{\alpha \boldsymbol{k} \sigma} \left( t_{\alpha\mu\boldsymbol{k}\sigma} a^\dagger_{\alpha\boldsymbol{k}\sigma} + t^*_{\alpha\mu\boldsymbol{k}\sigma} a_{\alpha\boldsymbol{k}\sigma} \right), \quad D_\mu = d_\mu + d^\dagger_\mu, \tag{4.6}$$

因而, 量子系统与电极的隧穿耦合项在相互作用绘景中可表示为

$$H_{\mathrm{T,I}}(t) = \sum_\mu D_\mu(t) F_{\alpha\mu}(t), \tag{4.7}$$

其中, $D_\mu(t)=\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}D_\mu\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}$, $F_{\alpha\mu}(t)=\mathrm{e}^{\mathrm{i}H_{\mathrm{leads}}t}F_{\alpha\mu}\mathrm{e}^{-\mathrm{i}H_{\mathrm{leads}}t}$, 并令

$$\hat{0}=D_i(t)\,,\quad \hat{1}=D_j(t_1)\,,\quad \hat{2}=D_k(t_2)\,,\quad \hat{3}=D_l(t_3)\,. \tag{4.8}$$

对于通常由式 (2.4) 描述的线性隧穿耦合项, 式 (4.7) 将简化为

$$H_{\mathrm{T}}=\sum_\mu\left(d_\mu(t)\,a^\dagger_{\alpha\mu}(t)+\mathrm{H.c.}\right), \tag{4.9}$$

其中, $d_\mu(t)=\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}d_\mu\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}$, $a^\dagger_{\alpha\mu}(t)=\sum\limits_{\alpha\boldsymbol{k}\sigma}t_{\alpha\mu\boldsymbol{k}\sigma}\mathrm{e}^{\mathrm{i}H_{\mathrm{leads}}t}a^\dagger_{\alpha\boldsymbol{k}\sigma}\mathrm{e}^{-\mathrm{i}H_{\mathrm{leads}}t}$. 将式 (4.7) 和式 (4.8) 代入式 (4.5) 可得

$$\begin{aligned}
K_4(t)\,P\rho_{\mathrm{I}}(t)\big|_{01}=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\Big\{\mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha i}(t)\,F_{\alpha j}(t_1)\,F_{\alpha k}(t_2)\,F_{\alpha l}(t_3)\,\rho_{\mathrm{leads}}\right]\hat{0}\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}(t)\\
&-\mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha i}(t)\,F_{\alpha j}(t_1)\,F_{\alpha k}(t_2)\,\rho_{\mathrm{leads}}F_{\alpha l}(t_3)\right]\hat{0}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}(t)\,\hat{3}\\
&-\mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha i}(t)\,F_{\alpha j}(t_1)\,F_{\alpha l}(t_3)\,\rho_{\mathrm{leads}}F_{\alpha k}(t_2)\right]\hat{0}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}(t)\,\hat{2}\\
&+\mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha i}(t)\,F_{\alpha j}(t_1)\,\rho_{\mathrm{leads}}F_{\alpha l}(t_3)\,F_{\alpha k}(t_2)\right]\hat{0}\hat{1}\rho_{\mathrm{QS,I}}(t)\,\hat{3}\hat{2}\\
&-\mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha i}(t)\,F_{\alpha k}(t_2)\,F_{\alpha l}(t_3)\,\rho_{\mathrm{leads}}F_{\alpha j}(t_1)\right]\hat{0}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}(t)\,\hat{1}\\
&+\mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha i}(t)\,F_{\alpha k}(t_2)\,\rho_{\mathrm{leads}}F_{\alpha l}(t_3)\,F_{\alpha j}(t_1)\right]\hat{0}\hat{2}\rho_{\mathrm{QS,I}}(t)\,\hat{3}\hat{1}\\
&+\mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha i}(t)\,F_{\alpha l}(t_3)\,\rho_{\mathrm{leads}}F_{\alpha k}(t_2)\,F_{\alpha j}(t_1)\right]\hat{0}\hat{3}\rho_{\mathrm{QS,I}}(t)\,\hat{2}\hat{1}\\
&-\mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha i}(t)\,\rho_{\mathrm{leads}}F_{\alpha l}(t_3)\,F_{\alpha k}(t_2)\,F_{\alpha j}(t_1)\right]\hat{0}\rho_{\mathrm{QS,I}}(t)\,\hat{3}\hat{2}\hat{1}\\
&-\mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha j}(t_1)\,F_{\alpha k}(t_2)\,F_{\alpha l}(t_3)\,\rho_{\mathrm{leads}}F_{\alpha i}(t)\right]\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}(t)\,\hat{0}\\
&+\mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha j}(t_1)\,F_{\alpha k}(t_2)\,\rho_{\mathrm{leads}}F_{\alpha l}(t_3)\,F_{\alpha i}(t)\right]\hat{1}\hat{2}\rho_{\mathrm{QS,I}}(t)\,\hat{3}\hat{0}\\
&+\mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha j}(t_1)\,F_{\alpha l}(t_3)\,\rho_{\mathrm{leads}}F_{\alpha k}(t_2)\,F_{\alpha i}(t)\right]\hat{1}\hat{3}\rho_{\mathrm{QS,I}}(t)\,\hat{2}\hat{0}\\
&-\mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha j}(t_1)\,\rho_{\mathrm{leads}}F_{\alpha l}(t_3)\,F_{\alpha k}(t_2)\,F_{\alpha i}(t)\right]\hat{1}\rho_{\mathrm{QS,I}}(t)\,\hat{3}\hat{2}\hat{0}\\
&+\mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha k}(t_2)\,F_{\alpha l}(t_3)\,\rho_{\mathrm{leads}}F_{\alpha j}(t_1)\,F_{\alpha i}(t)\right]\hat{2}\hat{3}\rho_{\mathrm{QS,I}}(t)\,\hat{1}\hat{0}\\
&-\mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha k}(t_2)\,\rho_{\mathrm{leads}}F_{\alpha l}(t_3)\,F_{\alpha j}(t_1)\,F_{\alpha i}(t)\right]\hat{2}\rho_{\mathrm{QS,I}}(t)\,\hat{3}\hat{1}\hat{0}\\
&-\mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha l}(t_3)\,\rho_{\mathrm{leads}}F_{\alpha k}(t_2)\,F_{\alpha j}(t_1)\,F_{\alpha i}(t)\right]\hat{3}\rho_{\mathrm{QS,I}}(t)\,\hat{2}\hat{1}\hat{0}\\
&+\mathrm{tr}_{\mathrm{leads}}\left[\rho_{\mathrm{leads}}F_{\alpha l}(t_3)\,F_{\alpha k}(t_2)\,F_{\alpha j}(t_1)\,F_{\alpha i}(t)\right]\rho_{\mathrm{QS,I}}(t)\,\hat{3}\hat{2}\hat{1}\hat{0}\Big\}\,,
\end{aligned} \tag{4.10}$$

由威克定理 (Wick theorem) 可知

$$\mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha i}(t)\,F_{\alpha j}(t_1)\,F_{\alpha k}(t_2)\,F_{\alpha l}(t_3)\,\rho_{\mathrm{leads}}\right]=C_{01}C_{23}+C_{02}C_{13}+C_{03}C_{12}, \tag{4.11}$$

其中

$$C_{01}= \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha i}\left(t\right)F_{\alpha j}\left(t_1\right)\rho_{\mathrm{leads}}\right], \tag{4.12}$$

$$C_{23}= \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha k}\left(t_2\right)F_{\alpha l}\left(t_3\right)\rho_{\mathrm{leads}}\right], \tag{4.13}$$

$$C_{02} = \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha i}\left(t\right)F_{\alpha k}\left(t_2\right)\rho_{\mathrm{leads}}\right], \tag{4.14}$$

$$C_{13}= \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha j}\left(t_1\right)F_{\alpha l}\left(t_3\right)\rho_{\mathrm{leads}}\right], \tag{4.15}$$

$$C_{03}= \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha i}\left(t\right)F_{\alpha l}\left(t_3\right)\rho_{\mathrm{leads}}\right], \tag{4.16}$$

$$C_{12}= \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha j}\left(t_1\right)F_{\alpha k}\left(t_2\right)\rho_{\mathrm{leads}}\right]. \tag{4.17}$$

利用求迹的性质, 可将式 (4.10) 重写为

$$\begin{aligned}
K_4\left(t\right)P\rho_{\mathrm{I}}\left(t\right)\big|_{01} = \sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 \\
&\times \Big\{\mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha i}\left(t\right)F_{\alpha j}\left(t_1\right)F_{\alpha k}\left(t_2\right)F_{\alpha l}\left(t_3\right)\rho_{\mathrm{leads}}\right]\hat{0}\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\left(t\right) \\
&- \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha l}\left(t_3\right)F_{\alpha i}\left(t\right)F_{\alpha j}\left(t_1\right)F_{\alpha k}\left(t_2\right)\rho_{\mathrm{leads}}\right]\hat{0}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\left(t\right)\hat{3} \\
&- \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha k}\left(t_2\right)F_{\alpha i}\left(t\right)F_{\alpha j}\left(t_1\right)F_{\alpha l}\left(t_3\right)\rho_{\mathrm{leads}}\right]\hat{0}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\left(t\right)\hat{2} \\
&+ \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha l}\left(t_3\right)F_{\alpha k}\left(t_2\right)F_{\alpha i}\left(t\right)F_{\alpha j}\left(t_1\right)\rho_{\mathrm{leads}}\right]\hat{0}\hat{1}\rho_{\mathrm{QS,I}}\left(t\right)\hat{3}\hat{2} \\
&- \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha j}\left(t_1\right)F_{\alpha i}\left(t\right)F_{\alpha k}\left(t_2\right)F_{\alpha l}\left(t_3\right)\rho_{\mathrm{leads}}\right]\hat{0}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\left(t\right)\hat{1} \\
&+ \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha l}\left(t_3\right)F_{\alpha j}\left(t_1\right)F_{\alpha i}\left(t\right)F_{\alpha k}\left(t_2\right)\rho_{\mathrm{leads}}\right]\hat{0}\hat{2}\rho_{\mathrm{QS,I}}\left(t\right)\hat{3}\hat{1} \\
&+ \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha k}\left(t_2\right)F_{\alpha j}\left(t_1\right)F_{\alpha i}\left(t\right)F_{\alpha l}\left(t_3\right)\rho_{\mathrm{leads}}\right]\hat{0}\hat{3}\rho_{\mathrm{QS,I}}\left(t\right)\hat{2}\hat{1} \\
&- \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha l}\left(t_3\right)F_{\alpha k}\left(t_2\right)F_{\alpha j}\left(t_1\right)F_{\alpha i}\left(t\right)\rho_{\mathrm{leads}}\right]\hat{0}\rho_{\mathrm{QS,I}}\left(t\right)\hat{3}\hat{2}\hat{1} \\
&- \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha i}\left(t\right)F_{\alpha j}\left(t_1\right)F_{\alpha k}\left(t_2\right)F_{\alpha l}\left(t_3\right)\rho_{\mathrm{leads}}\right]\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\left(t\right)\hat{0} \\
&+ \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha l}\left(t_3\right)F_{\alpha i}\left(t\right)F_{\alpha j}\left(t_1\right)F_{\alpha k}\left(t_2\right)\rho_{\mathrm{leads}}\right]\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\left(t\right)\hat{3}\hat{0} \\
&+ \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha k}\left(t_2\right)F_{\alpha i}\left(t\right)F_{\alpha j}\left(t_1\right)F_{\alpha l}\left(t_3\right)\rho_{\mathrm{leads}}\right]\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\left(t\right)\hat{2}\hat{0} \\
&- \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha l}\left(t_3\right)F_{\alpha k}\left(t_2\right)F_{\alpha i}\left(t\right)F_{\alpha j}\left(t_1\right)\rho_{\mathrm{leads}}\right]\hat{1}\rho_{\mathrm{QS,I}}\left(t\right)\hat{3}\hat{2}\hat{0} \\
&+ \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha j}\left(t_1\right)F_{\alpha i}\left(t\right)F_{\alpha k}\left(t_2\right)F_{\alpha l}\left(t_3\right)\rho_{\mathrm{leads}}\right]\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\left(t\right)\hat{1}\hat{0} \\
&- \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha l}\left(t_3\right)F_{\alpha j}\left(t_1\right)F_{\alpha i}\left(t\right)F_{\alpha k}\left(t_2\right)\rho_{\mathrm{leads}}\right]\hat{2}\rho_{\mathrm{QS,I}}\left(t\right)\hat{3}\hat{1}\hat{0} \\
&- \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha k}\left(t_2\right)F_{\alpha j}\left(t_1\right)F_{\alpha i}\left(t\right)F_{\alpha l}\left(t_3\right)\rho_{\mathrm{leads}}\right]\hat{3}\rho_{\mathrm{QS,I}}\left(t\right)\hat{2}\hat{1}\hat{0} \\
&+ \mathrm{tr}_{\mathrm{leads}}\left[F_{\alpha l}\left(t_3\right)F_{\alpha k}\left(t_2\right)F_{\alpha j}\left(t_1\right)F_{\alpha i}\left(t\right)\rho_{\mathrm{leads}}\right]\rho_{\mathrm{QS,I}}\left(t\right)\hat{3}\hat{2}\hat{1}\hat{0}\Big\},
\end{aligned} \tag{4.18}$$

对式 (4.18) 应用威克定理可得

$$
\begin{aligned}
K_4(t)\,P\rho_{\mathrm{I}}(t)\big|_{01} = \sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 \\
&\times\big[(C_{01}C_{23}+C_{02}C_{13}+C_{03}C_{12})\,\hat{0}\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}(t) \\
&-(C_{30}C_{12}+C_{31}C_{02}+C_{32}C_{01})\,\hat{0}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}(t)\,\hat{3} \\
&-(C_{20}C_{13}+C_{21}C_{03}+C_{23}C_{01})\,\hat{0}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}(t)\,\hat{2} \\
&+(C_{32}C_{01}+C_{30}C_{21}+C_{31}C_{20})\,\hat{0}\hat{1}\rho_{\mathrm{QS,I}}(t)\,\hat{3}\hat{2} \\
&-(C_{10}C_{23}+C_{12}C_{03}+C_{13}C_{02})\,\hat{0}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}(t)\,\hat{1} \\
&+(C_{31}C_{02}+C_{30}C_{12}+C_{32}C_{10})\,\hat{0}\hat{2}\rho_{\mathrm{QS,I}}(t)\,\hat{3}\hat{1} \\
&+(C_{21}C_{03}+C_{20}C_{13}+C_{23}C_{10})\,\hat{0}\hat{3}\rho_{\mathrm{QS,I}}(t)\,\hat{2}\hat{1} \\
&-(C_{32}C_{10}+C_{31}C_{20}+C_{30}C_{21})\,\hat{0}\rho_{\mathrm{QS,I}}(t)\,\hat{3}\hat{2}\hat{1} \\
&-(C_{01}C_{23}+C_{02}C_{13}+C_{03}C_{12})\,\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}(t)\,\hat{0} \\
&+(C_{30}C_{12}+C_{31}C_{02}+C_{32}C_{01})\,\hat{1}\hat{2}\rho_{\mathrm{QS,I}}(t)\,\hat{3}\hat{0} \\
&+(C_{20}C_{13}+C_{21}C_{03}+C_{23}C_{01})\,\hat{1}\hat{3}\rho_{\mathrm{QS,I}}(t)\,\hat{2}\hat{0} \\
&-(C_{32}C_{01}+C_{30}C_{21}+C_{31}C_{20})\,\hat{1}\rho_{\mathrm{QS,I}}(t)\,\hat{3}\hat{2}\hat{0} \\
&+(C_{10}C_{23}+C_{12}C_{03}+C_{13}C_{02})\,\hat{2}\hat{3}\rho_{\mathrm{QS,I}}(t)\,\hat{1}\hat{0} \\
&-(C_{31}C_{02}+C_{30}C_{12}+C_{32}C_{10})\,\hat{2}\rho_{\mathrm{QS,I}}(t)\,\hat{3}\hat{1}\hat{0} \\
&-(C_{21}C_{03}+C_{20}C_{13}+C_{23}C_{10})\,\hat{3}\rho_{\mathrm{QS,I}}(t)\,\hat{2}\hat{1}\hat{0} \\
&+(C_{32}C_{10}+C_{31}C_{20}+C_{30}C_{21})\,\rho_{\mathrm{QS,I}}(t)\,\hat{3}\hat{2}\hat{1}\hat{0}\big]\,, \qquad (4.19)
\end{aligned}
$$

将式 (4.19) 按照系数 $C_{01}(C_{10})$、$C_{02}(C_{20})$ 和 $C_{03}(C_{30})$ 整理成如下三项:

$$
\begin{aligned}
&K_4(t)\,P\rho_{\mathrm{I}}(t)\big|_{01-01} \\
&=\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 \\
&\times\big(C_{01}C_{23}\hat{0}\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}-C_{01}C_{23}\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{0}-C_{01}C_{32}\hat{0}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}+C_{01}C_{32}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{0} \\
&-C_{01}C_{23}\hat{0}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}+C_{01}C_{23}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{0}+C_{01}C_{32}\hat{0}\hat{1}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}-C_{01}C_{32}\hat{1}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}\hat{0} \\
&-C_{10}C_{23}\hat{0}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{1}+C_{10}C_{23}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{1}\hat{0}+C_{10}C_{32}\hat{0}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{1}-C_{10}C_{32}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{1}\hat{0} \\
&+C_{10}C_{23}\hat{0}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{1}-C_{10}C_{23}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{1}\hat{0}-C_{10}C_{32}\hat{0}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}\hat{1}+C_{10}C_{32}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}\hat{1}\hat{0}\big)\,,
\end{aligned}
\qquad (4.20)
$$

$$\begin{aligned}
&K_4(t)\,P\rho_{\mathrm{I}}(t)\big|_{01-02}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\big(C_{02}C_{13}\hat{0}\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}-C_{02}C_{13}\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{0}-C_{02}C_{31}\hat{0}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}+C_{02}C_{31}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{0}\\
&-C_{20}C_{13}\hat{0}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}+C_{20}C_{13}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{0}+C_{20}C_{31}\hat{0}\hat{1}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}-C_{20}C_{31}\hat{1}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}\hat{0}\\
&-C_{02}C_{13}\hat{0}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{1}+C_{02}C_{13}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{1}\hat{0}+C_{02}C_{31}\hat{0}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{1}-C_{02}C_{31}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{1}\hat{0}\\
&+C_{20}C_{13}\hat{0}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{1}-C_{20}C_{13}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{1}\hat{0}-C_{20}C_{31}\hat{0}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}\hat{1}+C_{20}C_{31}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}\hat{1}\hat{0}\big),
\end{aligned}\tag{4.21}$$

$$\begin{aligned}
&K_4(t)\,P\rho_{\mathrm{I}}(t)\big|_{01-03}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\big(C_{03}C_{12}\hat{0}\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}-C_{03}C_{12}\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{0}-C_{30}C_{12}\hat{0}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}+C_{30}C_{12}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{0}\\
&-C_{03}C_{21}\hat{0}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}+C_{03}C_{21}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{0}+C_{30}C_{21}\hat{0}\hat{1}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}-C_{30}C_{21}\hat{1}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}\hat{0}\\
&-C_{03}C_{12}\hat{0}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{1}+C_{03}C_{12}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{1}\hat{0}+C_{30}C_{12}\hat{0}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{1}-C_{30}C_{12}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{1}\hat{0}\\
&+C_{03}C_{21}\hat{0}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{1}-C_{03}C_{21}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{1}\hat{0}-C_{30}C_{21}\hat{0}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}\hat{1}+C_{30}C_{21}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}\hat{1}\hat{0}\big).
\end{aligned}\tag{4.22}$$

同理, 式 (4.2) 右边的第二项 $\sim$ 第四项可分别表示为

$$\begin{aligned}
&K_4(t)\,P\rho_{\mathrm{I}}(t)\big|_{02}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\big(-C_{01}C_{23}\hat{0}\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}+C_{01}C_{23}\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{0}+C_{01}C_{32}\hat{0}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}-C_{01}C_{32}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{0}\\
&+C_{01}C_{23}\hat{0}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}-C_{01}C_{23}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{0}-C_{01}C_{32}\hat{0}\hat{1}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}+C_{01}C_{32}\hat{1}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}\hat{0}\\
&+C_{10}C_{23}\hat{0}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{1}-C_{10}C_{23}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{1}\hat{0}-C_{10}C_{32}\hat{0}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{1}+C_{10}C_{32}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{1}\hat{0}\\
&-C_{10}C_{23}\hat{0}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{1}+C_{10}C_{23}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{1}\hat{0}+C_{10}C_{32}\hat{0}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}\hat{1}-C_{10}C_{32}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}\hat{1}\hat{0}\big),
\end{aligned}\tag{4.23}$$

$$\begin{aligned}
&K_4(t)\,P\rho_{\mathrm{I}}(t)\big|_{03}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\big(-C_{02}C_{13}\hat{0}\hat{2}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}+C_{02}C_{31}\hat{0}\hat{2}\hat{1}\rho_{\mathrm{QS,I}}\hat{3}+C_{02}C_{13}\hat{0}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{1}-C_{02}C_{31}\hat{0}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{1}\\
&+C_{20}C_{13}\hat{0}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}-C_{20}C_{31}\hat{0}\hat{1}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}-C_{20}C_{13}\hat{0}\hat{3}\rho_{\mathrm{QS,I}}\hat{1}\hat{2}+C_{20}C_{31}\hat{0}\rho_{\mathrm{QS,I}}\hat{3}\hat{1}\hat{2}
\end{aligned}$$

$$
\begin{aligned}
&+C_{02}C_{13}\hat{2}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\hat{0}-C_{02}C_{31}\hat{2}\hat{1}\rho_{\mathrm{QS,I}}\hat{3}\hat{0}-C_{02}C_{13}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{1}\hat{0}+C_{02}C_{31}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{1}\hat{0}\\
&-C_{20}C_{13}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{0}+C_{20}C_{31}\hat{1}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}\hat{0}+C_{20}C_{13}\hat{3}\rho_{\mathrm{QS,I}}\hat{1}\hat{2}\hat{0}-C_{20}C_{31}\rho_{\mathrm{QS,I}}\hat{3}\hat{1}\hat{2}\hat{0}\big)\,,
\end{aligned}
\tag{4.24}
$$

$$
\begin{aligned}
&K_4\left(t\right)P\rho_{\mathrm{I}}\left(t\right)\big|_{04}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\big(-C_{03}C_{12}\hat{0}\hat{3}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}+C_{03}C_{21}\hat{0}\hat{3}\hat{1}\rho_{\mathrm{QS,I}}\hat{2}+C_{03}C_{12}\hat{0}\hat{3}\hat{2}\rho_{\mathrm{QS,I}}\hat{1}-C_{03}C_{21}\hat{0}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{1}\\
&+C_{30}C_{12}\hat{0}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}-C_{30}C_{21}\hat{0}\hat{1}\rho_{\mathrm{QS,I}}\hat{2}\hat{3}-C_{30}C_{12}\hat{0}\hat{2}\rho_{\mathrm{QS,I}}\hat{1}\hat{3}+C_{30}C_{21}\hat{0}\rho_{\mathrm{QS,I}}\hat{2}\hat{1}\hat{3}\\
&+C_{03}C_{12}\hat{3}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\hat{0}-C_{03}C_{21}\hat{3}\hat{1}\rho_{\mathrm{QS,I}}\hat{2}\hat{0}-C_{03}C_{12}\hat{3}\hat{2}\rho_{\mathrm{QS,I}}\hat{1}\hat{0}+C_{03}C_{21}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{1}\hat{0}\\
&-C_{30}C_{12}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{0}+C_{30}C_{21}\hat{1}\rho_{\mathrm{QS,I}}\hat{2}\hat{3}\hat{0}+C_{30}C_{12}\hat{2}\rho_{\mathrm{QS,I}}\hat{1}\hat{3}\hat{0}-C_{30}C_{21}\rho_{\mathrm{QS,I}}\hat{2}\hat{1}\hat{3}\hat{0}\big)\,.
\end{aligned}
\tag{4.25}
$$

将式 (4.20) 加上式 (4.23) 可得

$$
K_4\left(t\right)P\rho_{\mathrm{I}}\left(t\right)\big|_{01-01}+K_4\left(t\right)P\rho_{\mathrm{I}}\left(t\right)\big|_{02}=0,
\tag{4.26}
$$

将式 (4.21) 加上式 (4.24) 可得

$$
\begin{aligned}
&K_4\left(t\right)P\rho_{\mathrm{I}}\left(t\right)\big|_{01-02}+K_4\left(t\right)P\rho_{\mathrm{I}}\left(t\right)\big|_{03}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\big(C_{02}C_{13}\hat{0}\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}-C_{02}C_{13}\hat{0}\hat{2}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}+C_{02}C_{13}\hat{2}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\hat{0}-C_{02}C_{13}\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{0}\\
&+C_{02}C_{31}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{0}-C_{02}C_{31}\hat{2}\hat{1}\rho_{\mathrm{QS,I}}\hat{3}\hat{0}+C_{02}C_{31}\hat{0}\hat{2}\hat{1}\rho_{\mathrm{QS,I}}\hat{3}-C_{02}C_{31}\hat{0}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\\
&+C_{20}C_{13}\hat{3}\rho_{\mathrm{QS,I}}\hat{1}\hat{2}\hat{0}-C_{20}C_{13}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{1}\hat{0}+C_{20}C_{13}\hat{0}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{1}-C_{20}C_{13}\hat{0}\hat{3}\rho_{\mathrm{QS,I}}\hat{1}\hat{2}\\
&+C_{20}C_{31}\hat{0}\rho_{\mathrm{QS,I}}\hat{3}\hat{1}\hat{2}-C_{20}C_{31}\hat{0}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}\hat{1}+C_{20}C_{31}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}\hat{1}\hat{0}-C_{20}C_{31}\rho_{\mathrm{QS,I}}\hat{3}\hat{1}\hat{2}\hat{0}\big)\,,
\end{aligned}
\tag{4.27}
$$

将式 (4.22) 加上式 (4.25) 可得

$$
\begin{aligned}
&K_4\left(t\right)P\rho_{\mathrm{I}}\left(t\right)\big|_{01-03}+K_4\left(t\right)P\rho_{\mathrm{I}}\left(t\right)\big|_{04}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\big(C_{03}C_{12}\hat{0}\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}-C_{03}C_{12}\hat{0}\hat{3}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}+C_{03}C_{12}\hat{3}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\hat{0}-C_{03}C_{12}\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{0}\\
&+C_{03}C_{12}\hat{0}\hat{3}\hat{2}\rho_{\mathrm{QS,I}}\hat{1}-C_{03}C_{12}\hat{0}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{1}+C_{03}C_{12}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{1}\hat{0}-C_{03}C_{12}\hat{3}\hat{2}\rho_{\mathrm{QS,I}}\hat{1}\hat{0}
\end{aligned}
$$

$$
\begin{aligned}
&+C_{03}C_{21}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{0}-C_{03}C_{21}\hat{3}\hat{1}\rho_{\mathrm{QS,I}}\hat{2}\hat{0}+C_{03}C_{21}\hat{0}\hat{3}\hat{1}\rho_{\mathrm{QS,I}}\hat{2}-C_{03}C_{21}\hat{0}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\\
&+C_{30}C_{12}\hat{0}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{1}-C_{30}C_{12}\hat{0}\hat{2}\rho_{\mathrm{QS,I}}\hat{1}\hat{3}+C_{30}C_{12}\hat{2}\rho_{\mathrm{QS,I}}\hat{1}\hat{3}\hat{0}-C_{30}C_{12}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{1}\hat{0}\\
&+C_{30}C_{21}\hat{0}\hat{1}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}-C_{30}C_{21}\hat{0}\hat{1}\rho_{\mathrm{QS,I}}\hat{2}\hat{3}+C_{30}C_{21}\hat{1}\rho_{\mathrm{QS,I}}\hat{2}\hat{3}\hat{0}-C_{30}C_{21}\hat{1}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}\hat{0}\\
&+C_{30}C_{21}\hat{0}\rho_{\mathrm{QS,I}}\hat{2}\hat{1}\hat{3}-C_{30}C_{21}\hat{0}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}\hat{1}+C_{30}C_{21}\rho_{\mathrm{QS,I}}\hat{3}\hat{2}\hat{1}\hat{0}-C_{30}C_{21}\rho_{\mathrm{QS,I}}\hat{2}\hat{1}\hat{3}\hat{0}\big).
\end{aligned}
\tag{4.28}
$$

利用算符对易关系的记号, 可将式 (4.27) 和式 (4.28) 进一步简写为

$$
\begin{aligned}
&K_4(t)\,P\rho_{\mathrm{I}}(t)\big|_{01-02}+K_4(t)\,P\rho_{\mathrm{I}}(t)\big|_{03}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\,\big(C_{02}C_{13}\big[\hat{0},\big[\hat{1},\hat{2}\big]\hat{3}\rho_{\mathrm{QS,I}}\big]-C_{02}C_{31}\big[\hat{0},\big[\hat{1},\hat{2}\big]\rho_{\mathrm{QS,I}}\hat{3}\big]\\
&-C_{20}C_{13}\big[\hat{0},\hat{3}\rho_{\mathrm{QS,I}}\big[\hat{1},\hat{2}\big]\big]+C_{20}C_{31}\big[\hat{0},\rho_{\mathrm{QS,I}}\hat{3}\big[\hat{1},\hat{2}\big]\big]\big),
\end{aligned}
\tag{4.29}
$$

$$
\begin{aligned}
&K_4(t)\,P\rho_{\mathrm{I}}(t)\big|_{01-03}+K_4(t)\,P\rho_{\mathrm{I}}(t)\big|_{04}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\,\big(C_{03}C_{12}\big[\hat{0},\big[\hat{1}\hat{2},\hat{3}\big]\rho_{\mathrm{QS,I}}\big]-C_{03}C_{12}\big[\hat{0},\big[\hat{2},\hat{3}\big]\rho_{\mathrm{QS,I}}\hat{1}\big]\\
&-C_{03}C_{21}\big[\hat{0},\big[\hat{1},\hat{3}\big]\rho_{\mathrm{QS,I}}\hat{2}\big]-C_{30}C_{12}\big[\hat{0},\hat{2}\rho_{\mathrm{QS,I}}\big[\hat{1},\hat{3}\big]\big]+C_{30}C_{21}\big[\hat{0},\rho_{\mathrm{QS,I}}\big[\hat{2}\hat{1},\hat{3}\big]\big]\\
&-C_{30}C_{21}\big[\hat{0},\hat{1}\rho_{\mathrm{QS,I}}\big[\hat{2},\hat{3}\big]\big]\big).
\end{aligned}
\tag{4.30}
$$

将式 (4.26)、(4.29) 和 (4.30) 代入式 (4.2) 可得

$$
\begin{aligned}
&K_4(t)\,P\rho_{\mathrm{I}}(t)\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\,\big(C_{02}C_{13}\big[\hat{0},\big[\hat{1},\hat{2}\big]\hat{3}\rho_{\mathrm{QS,I}}\big]-C_{02}C_{31}\big[\hat{0},\big[\hat{1},\hat{2}\big]\rho_{\mathrm{QS,I}}\hat{3}\big]\\
&-C_{20}C_{13}\big[\hat{0},\hat{3}\rho_{\mathrm{QS,I}}\big[\hat{1},\hat{2}\big]\big]+C_{20}C_{31}\big[\hat{0},\rho_{\mathrm{QS,I}}\hat{3}\big[\hat{1},\hat{2}\big]\big]+C_{03}C_{12}\big[\hat{0},\big[\hat{1}\hat{2},\hat{3}\big]\rho_{\mathrm{QS,I}}\big]\\
&-C_{03}C_{12}\big[\hat{0},\big[\hat{2},\hat{3}\big]\rho_{\mathrm{QS,I}}\hat{1}\big]-C_{03}C_{21}\big[\hat{0},\big[\hat{1},\hat{3}\big]\rho_{\mathrm{QS,I}}\hat{2}\big]-C_{30}C_{12}\big[\hat{0},\hat{2}\rho_{\mathrm{QS,I}}\big[\hat{1},\hat{3}\big]\big]\\
&+C_{30}C_{21}\big[\hat{0},\rho_{\mathrm{QS,I}}\big[\hat{2}\hat{1},\hat{3}\big]\big]-C_{30}C_{21}\big[\hat{0},\hat{1}\rho_{\mathrm{QS,I}}\big[\hat{2},\hat{3}\big]\big]\big)\otimes\rho_{\mathrm{leads}}.
\end{aligned}
\tag{4.31}
$$

另外, 由式 (2.129) 可知

$$
\begin{aligned}
&K_2(t)\,P\rho_{\mathrm{I}}(t)\\
=&-\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1\mathrm{tr}_{\mathrm{leads}}\left[H_{\mathrm{T,I}}(t)\,H_{\mathrm{T,I}}(t_1)\,\rho_{\mathrm{QS,I}}(t)\otimes\rho_{\mathrm{leads}}\right]\otimes\rho_{\mathrm{leads}}\\
&+\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1\mathrm{tr}_{\mathrm{leads}}\left[H_{\mathrm{T,I}}(t_1)\,\rho_{\mathrm{QS,I}}(t)\otimes\rho_{\mathrm{leads}}H_{\mathrm{T,I}}(t)\right]\otimes\rho_{\mathrm{leads}}\\
&+\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1\mathrm{tr}_{\mathrm{leads}}\left[H_{\mathrm{T,I}}(t)\,\rho_{\mathrm{QS,I}}(t)\otimes\rho_{\mathrm{leads}}H_{\mathrm{T,I}}(t_1)\right]\otimes\rho_{\mathrm{leads}}
\end{aligned}
$$

$$
\begin{aligned}
&-\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1\mathrm{tr}_{\mathrm{leads}}\left[\rho_{\mathrm{QS,I}}\left(t\right)\otimes\rho_{\mathrm{leads}}H_{\mathrm{T,I}}\left(t_1\right)H_{\mathrm{T,I}}\left(t\right)\right]\otimes\rho_{\mathrm{leads}}\\
&=\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1\left(-C_{01}\hat{0}\hat{1}\rho_{\mathrm{QS,I}}+C_{10}\hat{1}\rho_{\mathrm{QS,I}}\hat{0}+C_{01}\hat{0}\rho_{\mathrm{QS,I}}\hat{1}-C_{10}\rho_{\mathrm{QS,I}}\hat{1}\hat{0}\right)\otimes\rho_{\mathrm{leads}}\\
&=\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1\left[C_{01}\hat{0}\left(\rho_{\mathrm{QS,I}}\hat{1}-\hat{1}\rho_{\mathrm{QS,I}}\right)+C_{10}\left(\hat{1}\rho_{\mathrm{QS,I}}-\rho_{\mathrm{QS,I}}\hat{1}\right)\hat{0}\right]\otimes\rho_{\mathrm{leads}}\\
&=-\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1\left\{C_{01}\hat{0}\left[\hat{1},\rho_{\mathrm{QS,I}}\right]-C_{10}\left[\hat{1},\rho_{\mathrm{QS,I}}\right]\hat{0}\right\}\otimes\rho_{\mathrm{leads}},
\end{aligned}
\tag{4.32}
$$

因而, 在共隧穿极限下, 在相互作用绘景中, 开放量子系统约化密度矩阵的运动方程可以表示为 [1]

$$
\frac{\partial\rho_{\mathrm{QS,I}}\left(t\right)}{\partial t}=\left.\rho_{\mathrm{QS,I}}\left(t\right)\right|_{\text{second-order}}+\left.\rho_{\mathrm{QS,I}}\left(t\right)\right|_{\text{fourth-order}},\tag{4.33}
$$

其中

$$
\left.\rho_{\mathrm{QS,I}}\left(t\right)\right|_{\text{second-order}}=-\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1\left\{C_{01}\hat{0}\left[\hat{1},\rho_{\mathrm{QS,I}}\right]-C_{10}\left[\hat{1},\rho_{\mathrm{QS,I}}\right]\hat{0}\right\},\tag{4.34}
$$

$$
\begin{aligned}
&\left.\rho_{\mathrm{QS,I}}\left(t\right)\right|_{\text{fourth-order}}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\left(C_{02}C_{13}\left[\hat{0},\left[\hat{1},\hat{2}\right]\hat{3}\rho_{\mathrm{QS,I}}\right]-C_{02}C_{31}\left[\hat{0},\left[\hat{1},\hat{2}\right]\rho_{\mathrm{QS,I}}\hat{3}\right]\right.\\
&-C_{20}C_{13}\left[\hat{0},\hat{3}\rho_{\mathrm{QS,I}}\left[\hat{1},\hat{2}\right]\right]+C_{20}C_{31}\left[\hat{0},\rho_{\mathrm{QS,I}}\hat{3}\left[\hat{1},\hat{2}\right]\right]+C_{03}C_{12}\left[\hat{0},\left[\hat{1}\hat{2},\hat{3}\right]\rho_{\mathrm{QS,I}}\right]\\
&-C_{03}C_{12}\left[\hat{0},\left[\hat{2},\hat{3}\right]\rho_{\mathrm{QS,I}}\hat{1}\right]-C_{03}C_{21}\left[\hat{0},\left[\hat{1},\hat{3}\right]\rho_{\mathrm{QS,I}}\hat{2}\right]-C_{30}C_{12}\left[\hat{0},\hat{2}\rho_{\mathrm{QS,I}}\left[\hat{1},\hat{3}\right]\right]\\
&\left.+C_{30}C_{21}\left[\hat{0},\rho_{\mathrm{QS,I}}\left[\hat{2}\hat{1},\hat{3}\right]\right]-C_{30}C_{21}\left[\hat{0},\hat{1}\rho_{\mathrm{QS,I}}\left[\hat{2},\hat{3}\right]\right]\right).
\end{aligned}
\tag{4.35}
$$

## 4.2 四阶时间局域的量子主方程：薛定谔绘景

在本节中, 将推导在共隧穿极限下开放量子系统的约化密度矩阵在薛定谔绘景中的运动方程形式. 由于式 (4.33) 右边可以表示为

$$
\frac{\partial\rho_{\mathrm{QS,I}}\left(t\right)}{\partial t}=\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\left[\frac{\partial\rho_{\mathrm{QS}}\left(t\right)}{\partial t}+\mathrm{i}\left[H_{\mathrm{QS}},\rho_{\mathrm{QS}}\left(t\right)\right]\right]\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t},\tag{4.36}
$$

因而, 式 (4.33) 描述的开放量子系统约化密度矩阵的运动方程在薛定谔绘景中可表示为

$$
\frac{\partial\rho_{\mathrm{QS}}\left(t\right)}{\partial t}=-\mathrm{i}\left[H_{\mathrm{QS}},\rho_{\mathrm{QS}}\left(t\right)\right]
$$

$$+\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{second-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}+\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}. \tag{4.37}$$

由式 (4.34) 可知

$$\begin{aligned}&\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{second-order}}\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\\=&-\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1C_{01}\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}D_i\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t_1}D_j\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t_1}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS}}(t)\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\\&+\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1C_{10}\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t_1}D_j\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t_1}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS}}(t)\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}D_i\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\\&+\mathrm{H.c.},\end{aligned} \tag{4.38}$$

为方便推导, 做如下算符定义:

$$D_i=D_i^0, \tag{4.39}$$

$$\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}(t-t_1)}D_j\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_1)}=\mathrm{e}^{-\mathrm{i}L_{\mathrm{QS}}(t-t_1)}D_j=D_j^1, \tag{4.40}$$

$$\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}(t-t_2)}D_k\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_2)}=\mathrm{e}^{-\mathrm{i}L_{\mathrm{QS}}(t-t_2)}D_k=D_k^2, \tag{4.41}$$

$$\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}(t-t_3)}D_l\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_3)}=\mathrm{e}^{-\mathrm{i}L_{\mathrm{QS}}(t-t_3)}D_l=D_l^3. \tag{4.42}$$

此时, 式 (4.38) 可简化为

$$\begin{aligned}&\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{second-order}}\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\\=&\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1\left[-C_{01}D_i^0D_j^1\rho_{\mathrm{QS}}(t)+C_{10}D_j^1\rho_{\mathrm{QS}}(t)D_i^0\right]+\mathrm{H.c.},\end{aligned} \tag{4.43}$$

其中, 对于由式 (2.4) 描述的线性隧穿耦合项, 式 (4.43) 将展开为式 (2.159).

对于式 (4.37) 右边描述共隧穿过程的第三项, 利用式 (4.24) 和式 (4.25), 可将其简化为

$$\begin{aligned}&\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\\=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\big[C_{02}C_{13}\big(\hat{0}\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}-\hat{0}\hat{2}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\\&+\hat{2}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\hat{0}-\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{0}\big)\\&+C_{02}C_{31}\big(\hat{0}\hat{2}\hat{1}\rho_{\mathrm{QS,I}}\hat{3}-\hat{0}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}+\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\hat{3}\hat{0}-\hat{2}\hat{1}\rho_{\mathrm{QS,I}}\hat{3}\hat{0}\big)\\&+C_{03}C_{12}\big(\hat{0}\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}-\hat{0}\hat{3}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}+\hat{3}\hat{1}\hat{2}\rho_{\mathrm{QS,I}}\hat{0}-\hat{1}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{0}\big)\\&+C_{03}C_{12}\big(\hat{0}\hat{3}\hat{2}\rho_{\mathrm{QS,I}}\hat{1}-\hat{0}\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{1}+\hat{2}\hat{3}\rho_{\mathrm{QS,I}}\hat{1}\hat{0}-\hat{3}\hat{2}\rho_{\mathrm{QS,I}}\hat{1}\hat{0}\big)\\&+C_{03}C_{21}\big(\hat{0}\hat{3}\hat{1}\rho_{\mathrm{QS,I}}\hat{2}-\hat{0}\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}+\hat{1}\hat{3}\rho_{\mathrm{QS,I}}\hat{2}\hat{0}-\hat{3}\hat{1}\rho_{\mathrm{QS,I}}\hat{2}\hat{0}\big)+\mathrm{H.c.}\big]\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t},\end{aligned} \tag{4.44}$$

式 (4.44) 右边的五项可以分别展开为

$$\begin{aligned}
&\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{01}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3C_{02}C_{13}\left[D_i^0D_j^1D_k^2D_l^3\rho_{\mathrm{QS}}\left(t\right)-D_i^0D_k^2D_j^1D_l^3\rho_{\mathrm{QS}}\left(t\right)\right.\\
&\left.+D_k^2D_j^1D_l^3\rho_{\mathrm{QS}}\left(t\right)D_i^0-D_j^1D_k^2D_l^3\rho_{\mathrm{QS}}\left(t\right)D_i^0\right]+\mathrm{H.c.},
\end{aligned}\tag{4.45}$$

$$\begin{aligned}
&\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{02}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3C_{02}C_{31}\left[D_i^0D_k^2D_j^1\rho_{\mathrm{QS}}\left(t\right)D_l^3-D_i^0D_j^1D_k^2\rho_{\mathrm{QS}}\left(t\right)D_l^3\right.\\
&\left.+D_j^1D_k^2\rho_{\mathrm{QS}}\left(t\right)D_l^3D_i^0-D_k^2D_j^1\rho_{\mathrm{QS}}\left(t\right)D_l^3D_i^0\right]+\mathrm{H.c.},
\end{aligned}\tag{4.46}$$

$$\begin{aligned}
&\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{03}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3C_{03}C_{12}\left[D_i^0D_j^1D_k^2D_l^3\rho_{\mathrm{QS}}\left(t\right)-D_i^0D_l^3D_j^1D_k^2\rho_{\mathrm{QS}}\left(t\right)\right.\\
&\left.+D_l^3D_j^1D_k^2\rho_{\mathrm{QS}}\left(t\right)D_i^0-D_j^1D_k^2D_l^3\rho_{\mathrm{QS}}\left(t\right)D_i^0\right]+\mathrm{H.c.},
\end{aligned}\tag{4.47}$$

$$\begin{aligned}
&\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{04}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3C_{03}C_{12}\left[D_i^0D_l^3D_k^2\rho_{\mathrm{QS}}\left(t\right)D_j^1-D_i^0D_k^2D_l^3\rho_{\mathrm{QS}}\left(t\right)D_j^1\right.\\
&\left.+D_k^2D_l^3\rho_{\mathrm{QS}}\left(t\right)D_j^1D_i^0-D_l^3D_k^2\rho_{\mathrm{QS}}\left(t\right)D_j^1D_i^0\right]+\mathrm{H.c.},
\end{aligned}\tag{4.48}$$

$$\begin{aligned}
&\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{05}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3C_{03}C_{21}\left[D_i^0D_l^3D_j^1\rho_{\mathrm{QS}}\left(t\right)D_k^2-D_i^0D_j^1D_l^3\rho_{\mathrm{QS}}\left(t\right)D_k^2\right.\\
&\left.+D_j^1D_l^3\rho_{\mathrm{QS}}\left(t\right)D_k^2D_i^0-D_l^3D_j^1\rho_{\mathrm{QS}}\left(t\right)D_k^2D_i^0\right]+\mathrm{H.c.}.
\end{aligned}\tag{4.49}$$

因而, 开放量子系统约化密度矩阵在薛定谔绘景中的运动方程可表示为

$$\begin{aligned}
&\frac{\partial\rho_{\mathrm{QS,I}}\left(t\right)}{\partial t}\\
=&-\mathrm{i}\left[H_{\mathrm{QS}},\rho_{\mathrm{QS}}\left(t\right)\right]+\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1\left[-C_{01}D_i^0D_j^1\rho_{\mathrm{QS}}\left(t\right)+C_{10}D_j^1\rho_{\mathrm{QS}}\left(t\right)D_i^0\right]\\
&+\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3C_{02}C_{13}\left[D_i^0D_j^1D_k^2D_l^3\rho_{\mathrm{QS}}\left(t\right)-D_i^0D_k^2D_j^1D_l^3\rho_{\mathrm{QS}}\left(t\right)\right.\\
&\left.+D_k^2D_j^1D_l^3\rho_{\mathrm{QS}}\left(t\right)D_i^0-D_j^1D_k^2D_l^3\rho_{\mathrm{QS}}\left(t\right)D_i^0\right]
\end{aligned}$$

$$
\begin{aligned}
&+\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3C_{02}C_{31}\left[D_i^0D_k^2D_j^1\rho_{\mathrm{QS}}\left(t\right)D_l^3-D_i^0D_j^1D_k^2\rho_{\mathrm{QS}}\left(t\right)D_l^3\right.\\
&\left.+D_j^1D_k^2\rho_{\mathrm{QS}}\left(t\right)D_l^3D_i^0-D_k^2D_j^1\rho_{\mathrm{QS}}\left(t\right)D_l^3D_i^0\right]\\
&+\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3C_{03}C_{12}\left[D_i^0D_j^1D_k^2D_l^3\rho_{\mathrm{QS}}\left(t\right)-D_i^0D_l^3D_j^1D_k^2\rho_{\mathrm{QS}}\left(t\right)\right.\\
&\left.+D_l^3D_j^1D_k^2\rho_{\mathrm{QS}}\left(t\right)D_i^0-D_j^1D_k^2D_l^3\rho_{\mathrm{QS}}\left(t\right)D_i^0\right]\\
&+\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3C_{03}C_{12}\left[D_i^0D_l^3D_k^2\rho_{\mathrm{QS}}\left(t\right)D_j^1-D_i^0D_k^2D_l^3\rho_{\mathrm{QS}}\left(t\right)D_j^1\right.\\
&\left.+D_k^2D_l^3\rho_{\mathrm{QS}}\left(t\right)D_j^1D_i^0-D_l^3D_k^2\rho_{\mathrm{QS}}\left(t\right)D_j^1D_i^0\right]\\
&+\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3C_{03}C_{21}\left[D_i^0D_l^3D_j^1\rho_{\mathrm{QS}}\left(t\right)D_k^2-D_i^0D_j^1D_l^3\rho_{\mathrm{QS}}\left(t\right)D_k^2\right.\\
&\left.+D_j^1D_l^3\rho_{\mathrm{QS}}\left(t\right)D_k^2D_i^0-D_l^3D_j^1\rho_{\mathrm{QS}}\left(t\right)D_k^2D_i^0\right]+\mathrm{H.c.}.
\end{aligned}
\tag{4.50}
$$

## 4.3 四阶时间局域的粒子数分辨量子主方程

本节将基于式 (4.50) 给出, 在共隧穿极限下, 开放量子系统约化密度矩阵的粒子数分辨量子主方程. 若到 $t$ 时刻为止, 有 $n_{\mathrm{L}}$ 个电子隧穿到源极, 同时有 $n_{\mathrm{R}}$ 个电子隧穿到漏极, 相应的两个电极的希尔伯特子空间记为 $B^{(n_{\mathrm{L}},n_{\mathrm{R}})}(n_{\mathrm{L}}=0,1,2,\cdots;n_{\mathrm{R}}=0,1,2,\cdots)$. 因而, 两个电极的整个希尔伯特子空间可以表示成 $B=\oplus_{n_{\mathrm{L}},n_{\mathrm{R}}}B^{(n_{\mathrm{L}},n_{\mathrm{R}})}$. 此时, 式 (4.50) 关于对两个电极的整个希尔伯特空间平均需要替换为对其子空间的平均 [2]. 下面, 按照第 3 章描述的流程, 给出式 (4.50) 对应的粒子数分辨量子主方程.

对于量子系统与电极的隧穿耦合为式 (2.4) 描述的线性项, 有如下对应关系式:

$$C_{02}^{(+)}=\sum_{\alpha ik}\mathrm{tr}_{\mathrm{leads}}\left[a_{\alpha i}^{\dagger}\left(t\right)a_{\alpha k}\left(t_2\right)\rho_{\mathrm{leads}}\right],\quad D_i=d_i,D_k=d_k^{\dagger},\tag{4.51}$$

$$C_{02}^{(-)}=\sum_{\alpha ik}\mathrm{tr}_{\mathrm{leads}}\left[a_{\alpha i}\left(t\right)a_{\alpha k}^{\dagger}\left(t_2\right)\rho_{\mathrm{leads}}\right],\quad D_i=d_i^{\dagger},D_k=d_k,\tag{4.52}$$

$$C_{13}^{(+)}=\sum_{\alpha jl}\mathrm{tr}_{\mathrm{leads}}\left[a_{\alpha j}^{\dagger}\left(t_1\right)a_{\alpha l}\left(t_3\right)\rho_{\mathrm{leads}}\right],\quad D_j=d_j,D_l=d_l^{\dagger},\tag{4.53}$$

$$C_{13}^{(-)}=\sum_{\alpha jl}\mathrm{tr}_{\mathrm{leads}}\left[a_{\alpha j}\left(t_1\right)a_{\alpha l}^{\dagger}\left(t_3\right)\rho_{\mathrm{leads}}\right],\quad D_j=d_j^{\dagger},D_l=d_l,\tag{4.54}$$

$$C_{31}^{(+)}=\sum_{\alpha lj}\mathrm{tr}_{\mathrm{leads}}\left[a_{\alpha l}^{\dagger}\left(t_3\right)a_{\alpha j}\left(t_1\right)\rho_{\mathrm{leads}}\right],\quad D_l=d_l,D_j=d_j^{\dagger},\tag{4.55}$$

$$C_{31}^{(-)}=\sum_{\alpha lj}\mathrm{tr}_{\mathrm{leads}}\left[a_{\alpha l}\left(t_3\right)a_{\alpha j}^{\dagger}\left(t_1\right)\rho_{\mathrm{leads}}\right],\quad D_l=d_l^{\dagger},D_j=d_j,\tag{4.56}$$

$$C_{03}^{(+)}=\sum_{\alpha il}\mathrm{tr}_{\mathrm{leads}}\left[a_{\alpha i}^{\dagger}\left(t\right)a_{\alpha l}\left(t_3\right)\rho_{\mathrm{leads}}\right],\quad D_i=d_i,D_l=d_l^{\dagger},\tag{4.57}$$

$$C_{03}^{(-)}=\sum_{\alpha il}\mathrm{tr}_{\mathrm{leads}}\left[a_{\alpha i}\left(t\right)a_{\alpha l}^{\dagger}\left(t_3\right)\rho_{\mathrm{leads}}\right],\quad D_i=d_i^{\dagger},D_l=d_l,\tag{4.58}$$

$$C_{12}^{(+)}=\sum_{\alpha jk}\mathrm{tr}_{\mathrm{leads}}\left[a_{\alpha j}^{\dagger}\left(t_1\right)a_{\alpha k}\left(t_2\right)\rho_{\mathrm{leads}}\right],\quad D_j=d_j,D_k=d_k^{\dagger},\tag{4.59}$$

$$C_{12}^{(-)}=\sum_{\alpha jk}\mathrm{tr}_{\mathrm{leads}}\left[a_{\alpha j}\left(t_1\right)a_{\alpha k}^{\dagger}\left(t_2\right)\rho_{\mathrm{leads}}\right],\quad D_j=d_j^{\dagger},D_k=d_k,\tag{4.60}$$

$$C_{21}^{(+)}=\sum_{\alpha kj}\mathrm{tr}_{\mathrm{leads}}\left[a_{\alpha k}^{\dagger}\left(t_2\right)a_{\alpha j}\left(t_1\right)\rho_{\mathrm{leads}}\right],\quad D_k=d_k,D_j=d_j^{\dagger},\tag{4.61}$$

$$C_{21}^{(-)}=\sum_{\alpha kj}\mathrm{tr}_{\mathrm{leads}}\left[a_{\alpha k}\left(t_2\right)a_{\alpha j}^{\dagger}\left(t_1\right)\rho_{\mathrm{leads}}\right],\quad D_k=d_k^{\dagger},D_j=d_j.\tag{4.62}$$

为方便推导, 作如下算符定义:

$$d_i=d_{i,0},\tag{4.63}$$

$$d_i^{\dagger}=d_{i,0}^{\dagger},\tag{4.64}$$

$$\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}(t-t_1)}d_j\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_1)}=\mathrm{e}^{-\mathrm{i}L_{\mathrm{QS}}(t-t_1)}d_j=d_{j,1},\tag{4.65}$$

$$\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}(t-t_1)}d_j^{\dagger}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_1)}=\mathrm{e}^{-\mathrm{i}L_{\mathrm{QS}}(t-t_1)}d_j^{\dagger}=d_{j,1}^{\dagger},\tag{4.66}$$

$$\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}(t-t_2)}d_k\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_2)}=\mathrm{e}^{-\mathrm{i}L_{\mathrm{QS}}(t-t_2)}d_k=d_{k,2},\tag{4.67}$$

$$\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}(t-t_2)}d_k^{\dagger}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_2)}=\mathrm{e}^{-\mathrm{i}L_{\mathrm{QS}}(t-t_2)}d_k^{\dagger}=d_{k,2}^{\dagger},\tag{4.68}$$

$$\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}(t-t_3)}d_l\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_3)}=\mathrm{e}^{-\mathrm{i}L_{\mathrm{QS}}(t-t_3)}d_l=d_{l,3},\tag{4.69}$$

$$\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}(t-t_3)}d_l^{\dagger}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_3)}=\mathrm{e}^{-\mathrm{i}L_{\mathrm{QS}}(t-t_3)}d_l^{\dagger}=d_{l,3}^{\dagger}.\tag{4.70}$$

根据第 3 章标记开放量子系统条件性约化密度矩阵 $\rho_{\mathrm{QS}}^{(n)}(t)$ 和 $\rho_{\mathrm{QS}}^{(n\pm1)}(t)$ 的方法, 式 (4.50) 右边第二项描述电子顺序隧穿过程的条件性约化密度矩阵可表示为

$$\begin{aligned}
&\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1\left[-C_{01}D_i^0D_j^1\rho_{\mathrm{QS}}\left(t\right)+C_{10}D_j^1\rho_{\mathrm{QS}}\left(t\right)D_i^0+\mathrm{H.c.}\right]\Big|_{\mathrm{con}}\\
=&-\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1C_{01}^{(+)}d_{i,0}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}\left(t\right)-\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1C_{01}^{(-)}d_{i,0}^{\dagger}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}\left(t\right)\\
&+\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1C_{\mathrm{L}10}^{(+)}d_{i,0}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}\left(t\right)d_{j,1}+\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1C_{\mathrm{L}10}^{(-)}d_{i,0}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}\left(t\right)d_{j,1}^{\dagger}\\
&+\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1C_{\mathrm{R}10}^{(+)}d_{i,0}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}\left(t\right)d_{j,1}+\sum_{ij}\int_{t_0}^{t}\mathrm{d}t_1C_{\mathrm{R}10}^{(-)}d_{i,0}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}\left(t\right)d_{j,1}^{\dagger}
\end{aligned}$$

$$+\,\mathrm{H.c.}, \tag{4.71}$$

同样, 式 (4.50) 右边描述电子共隧穿过程的第三项, 即式 (4.45) 对应的条件性约化密度矩阵可表示为如下四项:

$$\begin{aligned}
&\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{01,\mathrm{con}}\Big|_{01}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\Big[C_{02}^{(-)}C_{13}^{(-)}d_{i,0}^{\dagger}d_{j,1}^{\dagger}d_{k,2}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)+C_{02}^{(-)}C_{13}^{(+)}d_{i,0}^{\dagger}d_{j,1}d_{k,2}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\\
&+C_{02}^{(+)}C_{13}^{(-)}d_{i,0}d_{j,1}^{\dagger}d_{k,2}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)+C_{02}^{(+)}C_{13}^{(+)}d_{i,0}d_{j,1}d_{k,2}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\Big]\\
&+\,\mathrm{H.c.},
\end{aligned} \tag{4.72}$$

$$\begin{aligned}
&\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{01,\mathrm{con}}\Big|_{02}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\Big[-C_{02}^{(-)}C_{13}^{(-)}d_{i,0}^{\dagger}d_{k,2}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)-C_{02}^{(-)}C_{13}^{(+)}d_{i,0}^{\dagger}d_{k,2}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\\
&-C_{02}^{(+)}C_{13}^{(-)}d_{i,0}d_{k,2}^{\dagger}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)-C_{02}^{(+)}C_{13}^{(+)}d_{i,0}d_{k,2}^{\dagger}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\Big]\\
&+\,\mathrm{H.c.},
\end{aligned} \tag{4.73}$$

$$\begin{aligned}
&\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{01,\mathrm{con}}\Big|_{03}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\Big[C_{\mathrm{L}02}^{(-)}C_{\mathrm{L}13}^{(-)}d_{k,2}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{i,0}^{\dagger}+C_{\mathrm{L}02}^{(-)}C_{\mathrm{R}13}^{(-)}d_{k,2}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{i,0}^{\dagger}\\
&+C_{\mathrm{L}02}^{(-)}C_{\mathrm{L}13}^{(+)}d_{k,2}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{i,0}^{\dagger}+C_{\mathrm{L}02}^{(-)}C_{\mathrm{R}13}^{(+)}d_{k,2}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{i,0}^{\dagger}\\
&+C_{\mathrm{R}02}^{(-)}C_{\mathrm{L}13}^{(-)}d_{k,2}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{i,0}^{\dagger}+C_{\mathrm{R}02}^{(-)}C_{\mathrm{R}13}^{(-)}d_{k,2}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{i,0}^{\dagger}\\
&+C_{\mathrm{R}02}^{(-)}C_{\mathrm{L}13}^{(+)}d_{k,2}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{i,0}^{\dagger}+C_{\mathrm{R}02}^{(-)}C_{\mathrm{R}13}^{(+)}d_{k,2}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{i,0}^{\dagger}\\
&+C_{\mathrm{L}02}^{(+)}C_{\mathrm{L}13}^{(-)}d_{k,2}^{\dagger}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{i,0}+C_{\mathrm{L}02}^{(+)}C_{\mathrm{R}13}^{(-)}d_{k,2}^{\dagger}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{i,0}\\
&+C_{\mathrm{L}02}^{(+)}C_{\mathrm{L}13}^{(+)}d_{k,2}^{\dagger}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{i,0}+C_{\mathrm{L}02}^{(+)}C_{\mathrm{R}13}^{(+)}d_{k,2}^{\dagger}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{i,0}\\
&+C_{\mathrm{R}02}^{(+)}C_{\mathrm{L}13}^{(-)}d_{k,2}^{\dagger}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{i,0}+C_{\mathrm{R}02}^{(+)}C_{\mathrm{R}13}^{(-)}d_{k,2}^{\dagger}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{i,0}\\
&+C_{\mathrm{R}02}^{(+)}C_{\mathrm{L}13}^{(+)}d_{k,2}^{\dagger}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{i,0}+C_{\mathrm{R}02}^{(+)}C_{\mathrm{R}13}^{(+)}d_{k,2}^{\dagger}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{i,0}\Big]\\
&+\,\mathrm{H.c.},
\end{aligned} \tag{4.74}$$

$$
\begin{aligned}
& \left.\left.\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\right|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\right|_{01,\mathrm{con}}\Big|_{04} \\
= & \sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 \\
& \times\Big[-C_{\mathrm{L02}}^{(-)}C_{\mathrm{L13}}^{(-)}d_{j,1}^{\dagger}d_{k,2}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{i,0}^{\dagger}-C_{\mathrm{L02}}^{(-)}C_{\mathrm{R13}}^{(-)}d_{j,1}^{\dagger}d_{k,2}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{i,0}^{\dagger} \\
& -C_{\mathrm{L02}}^{(-)}C_{\mathrm{L13}}^{(+)}d_{j,1}d_{k,2}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{i,0}^{\dagger}-C_{\mathrm{L02}}^{(-)}C_{\mathrm{R13}}^{(+)}d_{j,1}d_{k,2}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{i,0}^{\dagger} \\
& -C_{\mathrm{R02}}^{(-)}C_{\mathrm{L13}}^{(-)}d_{j,1}^{\dagger}d_{k,2}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{i,0}^{\dagger}-C_{\mathrm{R02}}^{(-)}C_{\mathrm{R13}}^{(-)}d_{j,1}^{\dagger}d_{k,2}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{i,0}^{\dagger} \\
& -C_{\mathrm{R02}}^{(-)}C_{\mathrm{L13}}^{(+)}d_{j,1}d_{k,2}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{i,0}^{\dagger}-C_{\mathrm{R02}}^{(-)}C_{\mathrm{R13}}^{(+)}d_{j,1}d_{k,2}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{i,0}^{\dagger} \\
& -C_{\mathrm{L02}}^{(+)}C_{\mathrm{L13}}^{(-)}d_{j,1}^{\dagger}d_{k,2}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{i,0}-C_{\mathrm{L02}}^{(+)}C_{\mathrm{R13}}^{(-)}d_{j,1}^{\dagger}d_{k,2}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{i,0} \\
& -C_{\mathrm{L02}}^{(+)}C_{\mathrm{L13}}^{(+)}d_{j,1}d_{k,2}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{i,0}-C_{\mathrm{L02}}^{(+)}C_{\mathrm{R13}}^{(+)}d_{j,1}d_{k,2}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{i,0} \\
& -C_{\mathrm{R02}}^{(+)}C_{\mathrm{L13}}^{(-)}d_{j,1}^{\dagger}d_{k,2}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{i,0}-C_{\mathrm{R02}}^{(+)}C_{\mathrm{R13}}^{(-)}d_{j,1}^{\dagger}d_{k,2}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{i,0} \\
& -C_{\mathrm{R02}}^{(+)}C_{\mathrm{L13}}^{(+)}d_{j,1}d_{k,2}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{i,0}-C_{\mathrm{R02}}^{(+)}C_{\mathrm{R13}}^{(+)}d_{j,1}d_{k,2}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{i,0}\Big] \\
& +\mathrm{H.c.},
\end{aligned}
\tag{4.75}
$$

同理, 可得式 (4.50) 中其余项对应的条件性约化密度矩阵, 其结果见附录 G. 因而, 在共隧穿极限下, 开放量子系统约化密度矩阵的时间局域粒子数分辨量子主方程可表示为 [3]

$$
\begin{aligned}
& \frac{\partial\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)}{\partial t} \\
= & -\mathrm{i}\left[H_{\mathrm{QS}},\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\right] \\
& +\left.\left.\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\right|_{\text{second-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\right|_{\mathrm{con}} \\
& +\sum_{m=1}^{5}\left.\left.\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\right|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\right|_{0m,\mathrm{con}}.
\end{aligned}
\tag{4.76}
$$

若只记录电子从所研究量子系统隧穿到漏极的电子数 $n$, 则上式形式上可简化为

$$
\begin{aligned}
& \frac{\partial\rho_{\mathrm{QS}}^{(n)}(t)}{\partial t} \\
& =A_0\rho_{\mathrm{QS}}^{(n)}(t)+B_{-1}\rho_{\mathrm{QS}}^{(n-1)}(t)+C_{+1}\rho_{\mathrm{QS}}^{(n+1)}(t) \\
& \quad+B_{-2}\rho_{\mathrm{QS}}^{(n-2)}(t)+C_{+2}\rho_{\mathrm{QS}}^{(n+2)}(t),
\end{aligned}
\tag{4.77}
$$

其中, $A_0$、$B_{-1}$、$C_{+1}$、$B_{-2}$ 和 $C_{+2}$ 是五个方阵. 需要说明的是, 方阵 $B_{-2}$ 和 $C_{+2}$ 描述的条件性约化密度矩阵仅由电子共隧穿引起.

## 4.4　共隧穿辅助顺序隧穿的电流高阶累积矩

在共隧穿极限下, 开放量子系统电流高阶累积矩的计算方法与第 3 章给出的顺序隧穿极限下的情形相同. 首先, 引入累积矩生成函数 $\mathrm{e}^{-F(\chi)}=\sum\limits_{n}P(n,t)\,\mathrm{e}^{\mathrm{i}n\chi}$, 并定义 $S(\chi,t)=\sum\limits_{n}\rho^{(n)}(t)\,\mathrm{e}^{\mathrm{i}n\chi}$, 因而有 $\mathrm{e}^{-F(\chi)}=\mathrm{tr}\,[S(\chi,t)]$. 对式 (4.77) 作分离傅里叶变换可得 $S(\chi,t)$ 满足：

$$\dot{S}=A_0S+\mathrm{e}^{\mathrm{i}\chi}B_{-1}S+\mathrm{e}^{-\mathrm{i}\chi}C_{+1}S+\mathrm{e}^{2\mathrm{i}\chi}B_{-2}S+\mathrm{e}^{-2\mathrm{i}\chi}C_{+2}S\equiv L(\chi)\,S. \tag{4.78}$$

在低频极限下, 计数时间 (即测量时间) 远大于电子通过开放量子系统的隧穿时间. 此时, $F(\chi)=-\lambda_0(\chi)\,t$, 其中, $\lambda_0(\chi)$ 是 $L(\chi)$ 的本征值, 且满足当 $\chi\to 0$ 时, 其数值趋于零. 根据累积矩的定义, $\lambda_0(\chi)$ 写成如下形式：

$$\lambda_0(\chi)=\sum_{k=1}^{\infty}\frac{C_k}{t}\frac{(\mathrm{i}\chi)^k}{k!}. \tag{4.79}$$

根据瑞利–薛定谔微扰理论, 可计算其电流的前四阶累积矩, 详见 3.4 节. 这里需要说明的是, 3.3 节给出的解析求解方法由于其符号计算的复杂性将不再适用.

### 参 考 文 献


[1] Breuer H P, Petruccione F. The Theory of Open Quantum Systems. Oxford: Oxford University Press, 2002: 450,451.

[2] Li X Q, Luo J Y, Yang Y G, et al. Quantum master-equation approach to quantum transport through mesoscopic systems. Phys. Rev. B, 2005, 71: 205304.

[3] Xue H B, Liang J Q, Liu W M. Non-Markovian full counting statistics of cotunneling assisted sequential tunneling in a side-coupled double quantum dot system. Physica E: Low-dimensional Systems and Nanostructures, 2019, 109: 39-51.

# 第 5 章　非马尔可夫电子计数统计理论的应用：顺序隧穿

在单分子和微纳器件的电子输运中, 电子的顺序隧穿过程是影响其输运特性的一个重要因素. 在本章中, 将基于二阶时间局域的粒子数分辨量子主方程, 以单量子点和耦合量子点为例, 给出其电子计数统计的计算流程, 并讨论其前四阶电流累积矩的特性, 最后, 给出在顺序隧穿极限下, 开放量子系统非马尔可夫电子计数统计与其系统量子相干性的关系.

## 5.1　引　　言

电子通过介观系统的电子计数统计 [1], 因其可以提供平均电流无法揭示的关于电子输运机制的本质信息, 引起了实验和理论的关注与研究兴趣 [2-11]. 例如, 散粒噪声的测量可以用来探测强相干耦合串联量子点的动力学特性 [12], 单量子点的近藤效应演化 [13], 以及量子导体的导体通道 [14]. 特别是, 散粒噪声的特性可以提供关于串联耦合量子点的赝自旋近藤效应特性 [15], 单电子库的自旋累积效应 [16], 以及量子霍尔边态 ($\nu = 2$) 的分数电荷 [17] 的信息. 此外, 双量子点中两个电子之间的纠缠自由度 [18], 单个封闭量子点中的退相位概率 [19], 单分子磁体的内部能级结构 [20,21] 可以用其超泊松分布的散粒噪声表征.

另一方面, 在密度矩阵理论中, 耦合量子点系统的量子相干性, 即量子点系统的约化密度矩阵的非对角元 [22], 在电子隧穿过程起重要作用并且对其电子输运性质有重要影响 [23-33]. 尤其是, 理论研究已经发现, 在不同类型的耦合量子点系统中, 相对于平均电流, 电流的高阶累积矩, 例如，散粒噪声和偏斜度, 更加敏感地依赖于其量子相干性 [12,34-38], 并且 T 型双量子点的量子相干性信息可以从其高阶累积矩特性中提取 [35]. 事实上, 量子系统的非马尔可夫动力学特性在电子的非平衡隧穿过程中也起着重要作用. 但是, 上面关于电流噪声和电子计数统计的研究主要基于不同类型的马尔可夫量子主方程. 虽然量子点系统的非马尔可夫效应对其在长时间极限下的电子计数统计特性已引起一些研究 [33,39-46], 但是, 非马尔可夫效应如何影响电子的计数统计依然是一个开放的课题. 特别是, 非马尔可夫效应和量子相干性对长时间极限下电子计数统计特性的影响尚未被揭示.

在本章中, 基于时间局域的粒子数分辨量子主方程, 以无量子相干性的单量子

点、串联耦合双量子点以及 T 型双量子点为例, 主要研究量子点系统的非马尔可夫效应和量子相干性对其电子计数统计特性的影响. 这里需要说明的是, 在下面的数值结果中, 与非马尔可夫情形下作对比的马尔可夫情形下的电子计数统计, 是基于忽略电子库谱函数虚部的马尔可夫粒子数分辨量子主方程, (式 (2.101)) 的数值结果 [47,48]. 为方便讨论, 下面讨论三种典型的量子点系统: 无量子相干性的单量子点系统, 量子相干性可调的串联耦合双量子点和 T 型双量子点, 如图 5.1 所示. 另外, 假设偏置电压对称地加载到由量子点和电极形成的隧穿结上, 即量子点系统的能级不依赖于外加的偏置电压, 即使在量子点与源极、漏极的隧穿耦合不对称时, 量子点系统的能级也不依赖于外加的偏置电压.

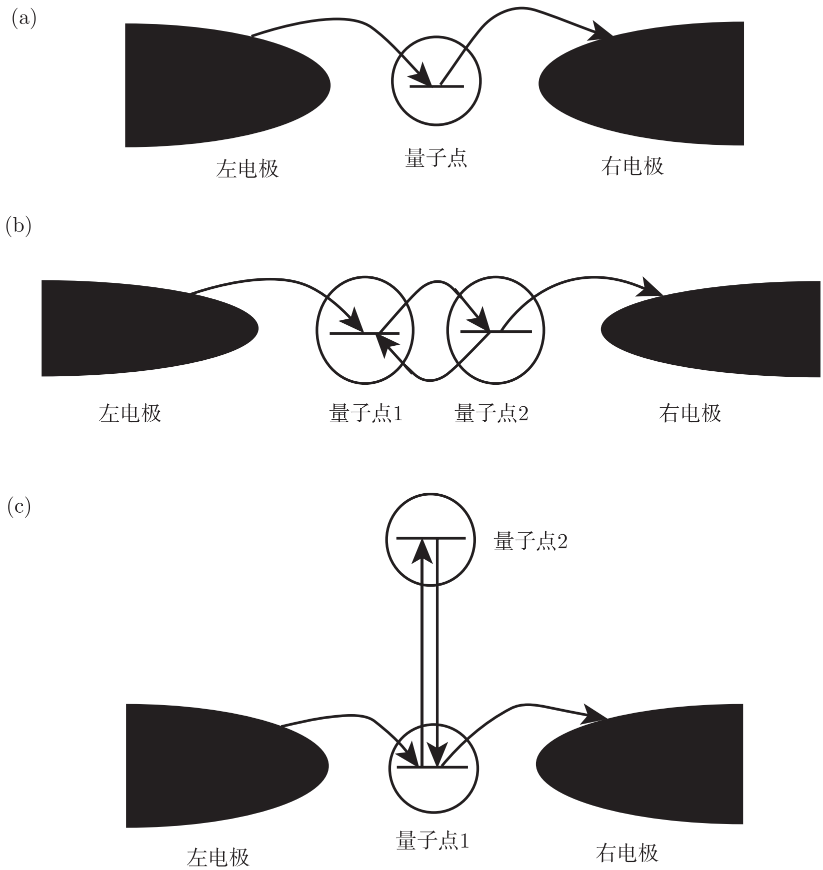


图 5.1 本章考虑的三个典型的开放量子点系统. (a) 无量子相干性的单能级单量子点; (b) 量子相干性可调的串联耦合双量子点; (c) 量子相干性可调的 T 型双量子点

## 5.2 无量子相干性的单量子点

在密度矩阵理论中, 当量子点系统的约化密度矩阵元无非对角项时, 该系统无量子相干性. 为此, 在本小节中, 考虑由一个单能级单量子点与两个自旋极化方向平行的铁磁电极耦合的开放量子系统.

### 5.2.1 开放单量子点系统的哈密顿量

一个单能级单量子点与两个电极耦合的开放量子系统的哈密顿量可以表示为

$$H = H_{\mathrm{dot},1} + H_{\mathrm{leads},1} + H_{\mathrm{tun},1}, \tag{5.1}$$

式 (5.1) 中的第一项为单能级单量子点的哈密顿量, 即

$$H_{\mathrm{dot},1} = \sum_{\sigma=\uparrow,\downarrow} \varepsilon_\sigma d_\sigma^\dagger d_\sigma + U d_\uparrow^\dagger d_\uparrow d_\downarrow^\dagger d_\downarrow, \tag{5.2}$$

其中, $d_\sigma^\dagger\,(d_\sigma)$ 表示在量子点能量为 $\varepsilon_\sigma$ 的能级上产生 (湮灭) 一个自旋为 $\sigma$ 的电子, $U$ 表示在能级 $\varepsilon_\sigma$ 上两个电子之间的库仑相互作用. 式 (5.1) 中的第二项 $H_{\mathrm{leads},1}$ 为两个铁磁电极 (电子库) 的哈密顿量. 若两个铁磁电极的电子弛豫过程足够快, 则其电子分布可以用平衡态的费米分布函数描述, 因而, 两个铁磁电极的哈密顿量可以表示为

$$H_{\mathrm{leads},1} = \sum_{\alpha\boldsymbol{k}s} \varepsilon_{\alpha\boldsymbol{k}} a_{\alpha\boldsymbol{k}s}^\dagger a_{\alpha\boldsymbol{k}s}, \tag{5.3}$$

其中, $a_{\alpha\boldsymbol{k}s}^\dagger\,(a_{\alpha\boldsymbol{k}s})$ 表示在 $\alpha(\alpha=\mathrm{L},\mathrm{R})$ 电极上产生 (湮灭) 一个自旋为 $s$、能量为 $\varepsilon_{\alpha\boldsymbol{k}}$、动量为 $k$ 的电子; $s=+(-)$ 表示铁磁电极的多数 (少数) 自旋态, 其态密度记为 $g_{\alpha,s}$. 此外, 由于左右铁磁电极的极化矢量 $\boldsymbol{p}_{\mathrm{L}}$ 和 $\boldsymbol{p}_{\mathrm{R}}$ 相互平行, 其电极极化率的大小可以表示为

$$p_\alpha = |\boldsymbol{p}_\alpha| = \frac{g_{\alpha,+} - g_{\alpha,-}}{g_{\alpha,+} + g_{\alpha,-}}. \tag{5.4}$$

相应地, 单量子点与左右铁磁电极的隧穿耦合, 即式 (5.1) 中的第三项 $H_{\mathrm{tun},1}$ 可表示为

$$H_{\mathrm{tun},1} = t_{\mathrm{L}\boldsymbol{k}+} a_{\mathrm{L}\boldsymbol{k}+}^\dagger d_\uparrow + t_{\mathrm{R}\boldsymbol{k}+} a_{\mathrm{R}\boldsymbol{k}+}^\dagger d_\uparrow + t_{\mathrm{L}\boldsymbol{k}-} a_{\mathrm{L}\boldsymbol{k}-}^\dagger d_\downarrow + t_{\mathrm{R}\boldsymbol{k}-} a_{\mathrm{R}\boldsymbol{k}-}^\dagger d_\downarrow + \mathrm{H.c.}, \tag{5.5}$$

其中, 量子点的自旋量子化轴选取为铁磁电极的电子极化方向, 因而, 量子点中电子的自旋向上 (即 $\sigma=\uparrow$) 和自旋向下 (即 $\sigma=\downarrow$) 的状态分别对应于铁磁电极中的多数自旋态和少数自旋态的情形.

### 5.2.2 单量子点的时间局域量子主方程

对于量子点与源极、漏极之间的隧穿耦合强度为弱耦合的情形, 电子的顺序隧穿占主要地位, 该过程可以用量子点本征态张开的约化密度矩阵的二阶时间局域量子主方程描述. 相应地, 单量子点约化密度矩阵的时间局域的粒子数分辨量子主方程可以表示为

$$\begin{aligned}\frac{\mathrm{d}\rho_{\mathrm{dot},1}^{(n)}}{\mathrm{d}t} =& -\mathrm{i}\left[H_{\mathrm{dot},1},\rho_{\mathrm{dot},1}^{(n)}\right] - \sum_{\sigma}\Bigg[d_{\sigma}^{\dagger}A_{\mathrm{L}\sigma}^{(-)}\left(L_{\mathrm{dot},1}\right)\rho_{\mathrm{dot},1}^{(n)} + d_{\sigma}^{\dagger}A_{\mathrm{R}\sigma}^{(-)}\left(L_{\mathrm{dot},1}\right)\rho_{\mathrm{dot},1}^{(n)}\\ &+ \rho_{\mathrm{dot},1}^{(n)}A_{\mathrm{L}\sigma}^{(+)}\left(L_{\mathrm{dot},1}\right)d_{\sigma}^{\dagger} + \rho_{\mathrm{dot},1}^{(n)}A_{\mathrm{R}\sigma}^{(+)}\left(L_{\mathrm{dot},1}\right)d_{\sigma}^{\dagger}\\ &- d_{\sigma}^{\dagger}\rho_{\mathrm{dot},1}^{(n)}A_{\mathrm{L}\sigma}^{(+)}\left(L_{\mathrm{dot},1}\right) - d_{\sigma}^{\dagger}\rho_{\mathrm{dot},1}^{(n+1)}A_{\mathrm{R}\sigma}^{(+)}\left(\mathrm{L}_{\mathrm{dot},1}\right)\\ &- A_{\mathrm{L}\sigma}^{(-)}\left(L_{\mathrm{dot},1}\right)\rho_{\mathrm{dot},1}^{(n)}d_{\sigma}^{\dagger} - A_{\mathrm{R}\sigma}^{(-)}\left(L_{\mathrm{dot},1}\right)\rho_{\mathrm{dot},1}^{(n-1)}d_{\sigma}^{\dagger} + \mathrm{H.c.}\Bigg],\end{aligned} \tag{5.6}$$

其中, 超算符和隧穿概率 $\Gamma_{\alpha\sigma}$ 定义为

$$A_{\alpha\sigma}^{(\pm)}\left(L_{\mathrm{dot},1}\right) = \frac{\Gamma_{\alpha\sigma}}{2\pi}\int\mathrm{d}\omega\int_{-\infty}^{t}\mathrm{d}t_1 g_{\alpha}\left(\omega\right)f_{\alpha}^{(\pm)}\left(\omega\right)\mathrm{e}^{-\mathrm{i}\left(\omega+L_{\mathrm{dot},1}\right)\left(t-t_1\right)}d_{\sigma}, \tag{5.7}$$

$$\Gamma_{\alpha\sigma} = 2\pi g_{\alpha,\sigma}\left|t_{\alpha\sigma}\right|^2, \tag{5.8}$$

这里, 已选取 $\hbar\equiv 1$. 为计算单量子点约化密度矩阵的矩阵元运动方程, 选取单量子点的四个电子状态: $|0,0\rangle$, $|\uparrow,0\rangle$, $|0,\downarrow\rangle$, $|\uparrow,\downarrow\rangle$ 为完备基对角化单量子点的哈密顿量, 即式 (5.2), 相应地, 其本征态和本征值可表示为

$$H_{\mathrm{dot},1}\left|0,0\right\rangle = \varepsilon_0\left|0,0\right\rangle, \quad \varepsilon_0 = 0, \tag{5.9}$$

$$H_{\mathrm{dot},1}\left|\uparrow,0\right\rangle = \varepsilon_{\uparrow}\left|\uparrow,0\right\rangle, \tag{5.10}$$

$$H_{\mathrm{dot},1}\left|0,\downarrow\right\rangle = \varepsilon_{\downarrow}\left|0,\downarrow\right\rangle, \tag{5.11}$$

$$H_{\mathrm{dot},1}\left|\uparrow,\downarrow\right\rangle = \varepsilon_{\uparrow,\downarrow}\left|0,0\right\rangle, \quad \varepsilon_{\uparrow,\downarrow} = \varepsilon_{\uparrow}+\varepsilon_{\downarrow}+U. \tag{5.12}$$

下面计算单量子点约化密度矩阵的矩阵元 $\rho_{\mathrm{dot},1,00}^{(n)} = \left\langle 0,0\right|\rho_{\mathrm{dot},1}^{(n)}\left|0,0\right\rangle$ 的运动方程 $\dot{\rho}_{\mathrm{dot},1,00}^{(n)}$, 将式 (5.9) 代入式 (5.6) 可得

$$\begin{aligned}\dot{\rho}_{\mathrm{dot},1,00}^{(n)} = \sum_{\sigma}\Bigg[&-\left\langle 0,0\right|\rho_{\mathrm{dot},1}^{(n)}A_{\mathrm{L}\sigma}^{(+)}\left(L_{\mathrm{dot},1}\right)d_{\sigma}^{\dagger}\left|0,0\right\rangle\\ &-\left\langle 0,0\right|\rho_{\mathrm{dot},1}^{(n)}A_{\mathrm{R}\sigma}^{(+)}\left(L_{\mathrm{dot},1}\right)d_{\sigma}^{\dagger}\left|0,0\right\rangle\\ &+\left\langle 0,0\right|A_{\mathrm{L}\sigma}^{(-)}\left(L_{\mathrm{dot},1}\right)\rho_{\mathrm{dot},1}^{(n)}d_{\sigma}^{\dagger}\left|0,0\right\rangle\end{aligned}$$

$$+\left\langle 0,0\right| A_{\mathrm{R}\sigma}^{(-)}\left(L_{\mathrm{dot},1}\right)\rho_{\mathrm{dot},1}^{(n-1)}d_{\sigma}^{\dagger}\left|0,0\right\rangle+\mathrm{H.c.}\Big], \tag{5.13}$$

将式 (5.13) 展开可得

$$\begin{aligned}
&\dot{\rho}_{\mathrm{dot},1,00}^{(n)}\\
=&-\left\langle 0,0\right|\rho_{\mathrm{dot},1}^{(n)}A_{\mathrm{L}\uparrow}^{(+)}\left(L_{\mathrm{dot},1}\right)\left|\uparrow,0\right\rangle-\left\langle 0,0\right|\rho_{\mathrm{dot},1}^{(n)}A_{\mathrm{R}\uparrow}^{(+)}\left(L_{\mathrm{dot},1}\right)\left|\uparrow,0\right\rangle\\
&-\left\langle 0,0\right|\rho_{\mathrm{dot},1}^{(n)}A_{\mathrm{L}\downarrow}^{(+)}\left(L_{\mathrm{dot},1}\right)\left|0,\downarrow\right\rangle-\left\langle 0,0\right|\rho_{\mathrm{dot},1}^{(n)}A_{\mathrm{R}\downarrow}^{(+)}\left(L_{\mathrm{dot},1}\right)\left|0,\downarrow\right\rangle\\
&+\left\langle 0,0\right| A_{\mathrm{L}\uparrow}^{(-)}\left(L_{\mathrm{dot},1}\right)\rho_{\mathrm{dot},1}^{(n)}\left|\uparrow,0\right\rangle+\left\langle 0,0\right| A_{\mathrm{R}\uparrow}^{(-)}\left(L_{\mathrm{dot},1}\right)\rho_{\mathrm{dot},1}^{(n-1)}\left|\uparrow,0\right\rangle\\
&+\left\langle 0,0\right| A_{\mathrm{L}\downarrow}^{(-)}\left(L_{\mathrm{dot},1}\right)\rho_{\mathrm{dot},1}^{(n)}\left|0,\downarrow\right\rangle+\left\langle 0,0\right| A_{\mathrm{R}\downarrow}^{(-)}\left(L_{\mathrm{dot},1}\right)\rho_{\mathrm{dot},1}^{(n-1)}\left|0,\downarrow\right\rangle\\
&-\left\langle 0,\uparrow\right|\left[A_{\mathrm{L}\uparrow}^{(+)}\left(L_{\mathrm{dot},1}\right)\right]^{\dagger}\rho_{\mathrm{dot},1}^{(n)}\left|0,0\right\rangle-\left\langle 0,\uparrow\right|\left[A_{\mathrm{R}\sigma}^{(+)}\left(L_{\mathrm{dot},1}\right)\right]^{\dagger}\rho_{\mathrm{dot},1}^{(n)}\left|0,0\right\rangle\\
&-\left\langle \downarrow,0\right|\left[A_{\mathrm{L}\downarrow}^{(+)}\left(L_{\mathrm{dot},1}\right)\right]^{\dagger}\rho_{\mathrm{dot},1}^{(n)}\left|0,0\right\rangle-\left\langle \downarrow,0\right|\left[A_{\mathrm{R}\downarrow}^{(+)}\left(L_{\mathrm{dot},1}\right)\right]^{\dagger}\rho_{\mathrm{dot},1}^{(n)}\left|0,0\right\rangle\\
&+\left\langle 0,\uparrow\right|\rho_{\mathrm{dot},1}^{(n)}\left[A_{\mathrm{L}\uparrow}^{(-)}\left(L_{\mathrm{dot},1}\right)\right]^{\dagger}\left|0,0\right\rangle+\left\langle 0,\uparrow\right|\rho_{\mathrm{dot},1}^{(n-1)}\left[A_{\mathrm{R}\uparrow}^{(-)}\left(L_{\mathrm{dot},1}\right)\right]^{\dagger}\left|0,0\right\rangle\\
&+\left\langle \downarrow,0\right|\rho_{\mathrm{dot},1}^{(n)}\left[A_{\mathrm{L}\downarrow}^{(-)}\left(L_{\mathrm{dot},1}\right)\right]^{\dagger}\left|0,0\right\rangle+\left\langle \downarrow,0\right|\rho_{\mathrm{dot},1}^{(n-1)}\left[A_{\mathrm{R}\downarrow}^{(-)}\left(L_{\mathrm{dot},1}\right)\right]^{\dagger}\left|0,0\right\rangle,
\end{aligned} \tag{5.14}$$

为了计算式 (5.14), 需要对式 (5.7) 求关于时间 $t_1$ 的积分, 其结果可表示为

$$A_{\alpha\sigma}^{(\pm)}\left(L_{\mathrm{dot},1}\right)=\frac{\mathrm{i}\Gamma_{\alpha\sigma}}{2\pi}\int\mathrm{d}\omega\frac{g_{\alpha}\left(\omega\right)f_{\alpha}^{(\pm)}\left(\omega\right)}{\mathrm{i}\eta-\omega-L_{\mathrm{dot},1}}d_{\sigma}, \tag{5.15}$$

$$\begin{aligned}
\left[A_{\alpha\sigma}^{(\pm)}\left(L_{\mathrm{dot},1}\right)\right]^{\dagger}=&\frac{\Gamma_{\alpha\sigma}}{2\pi}\int\mathrm{d}\omega\int_{-\infty}^{t}\mathrm{d}t_1 g_{\alpha}\left(\omega\right)f_{\alpha}^{(\pm)}\left(\omega\right)\mathrm{e}^{\mathrm{i}\left(\omega-L_{\mathrm{dot},1}\right)\left(t-t_1\right)}d_{\sigma}^{\dagger}\\
=&\frac{\mathrm{i}\Gamma_{\alpha\sigma}}{2\pi}\int\mathrm{d}\omega\frac{g_{\alpha}\left(\omega\right)f_{\alpha}^{(\pm)}\left(\omega\right)}{\mathrm{i}\eta+\omega-L_{\mathrm{dot},1}}d_{\sigma}^{\dagger}.
\end{aligned} \tag{5.16}$$

其中, $\eta\to 0^{+}$. 此外, 由附录 B 的式 (B.12)、(B.14)、(B.22)、(B.24) 可知,

$$\left\langle m\right|\left[f\left(L_{\mathrm{dot},1}\right)d_{\mu'}\right]\rho_{\mathrm{dot},1}\left|n\right\rangle=f\left(\varepsilon_m-\varepsilon_{m'}\right)\left\langle m'\right|\rho_{\mathrm{dot},1}\left|n\right\rangle,\quad \left\langle m\right|d_{\mu'}=\left\langle m'\right|, \tag{5.17}$$

$$\left\langle m\right|\left[f\left(L_{\mathrm{dot},1}\right)d_{\mu'}^{\dagger}\right]\rho_{\mathrm{dot},1}\left|n\right\rangle=f\left(\varepsilon_m-\varepsilon_{m''}\right)\left\langle m''\right|\rho_{\mathrm{dot},1}\left|n\right\rangle,\quad \left\langle m\right|d_{\mu'}^{\dagger}=\left\langle m''\right|, \tag{5.18}$$

$$\left\langle m\right|\rho_{\mathrm{dot},1}\left[f\left(L_{\mathrm{dot},1}\right)d_{\mu'}\right]\left|n\right\rangle=f\left(\varepsilon_{n'}-\varepsilon_n\right)\left\langle m\right|\rho_{\mathrm{dot},1}\left|n'\right\rangle,\quad d_{\mu'}\left|n\right\rangle=\left|n'\right\rangle, \tag{5.19}$$

$$\left\langle m\right|\rho_{\mathrm{dot},1}\left[f\left(L_{\mathrm{dot},1}\right)d_{\mu'}^{\dagger}\right]\left|n\right\rangle=f\left(\varepsilon_{n''}-\varepsilon_n\right)\left\langle m\right|\rho_{\mathrm{dot},1}\left|n''\right\rangle,\quad d_{\mu'}^{\dagger}\left|n\right\rangle=\left|n''\right\rangle. \tag{5.20}$$

其中, $f\left(L_{\mathrm{dot},1}\right)$ 是关于 $L_{\mathrm{dot},1}$ 的函数. 将式 (5.15)∼ 式 (5.20) 代入式 (5.14) 可得

$$\begin{aligned}
\dot{\rho}_{\mathrm{dot},1,00}^{(n)}= & -\frac{\mathrm{i}\Gamma_{\mathrm{L}\uparrow}}{2\pi}\left[I_{1,\mathrm{L}+}\left(\varepsilon_{\uparrow}\right)+I_{2,\mathrm{L}+}\left(\varepsilon_{\uparrow}\right)\right]\rho_{\mathrm{dot},1,00}^{(n)} \\
& -\frac{\mathrm{i}\Gamma_{\mathrm{R}\uparrow}}{2\pi}\left[I_{1,\mathrm{R}+}\left(\varepsilon_{\uparrow}\right)+I_{2,\mathrm{R}+}\left(\varepsilon_{\uparrow}\right)\right]\rho_{\mathrm{dot},1,00}^{(n)} \\
& -\frac{\mathrm{i}\Gamma_{\mathrm{L}\downarrow}}{2\pi}\left[I_{1,\mathrm{L}+}\left(\varepsilon_{\downarrow}\right)+I_{2,\mathrm{L}+}\left(\varepsilon_{\downarrow}\right)\right]\rho_{\mathrm{dot},1,00}^{(n)} \\
& -\frac{\mathrm{i}\Gamma_{\mathrm{R}\downarrow}}{2\pi}\left[I_{1,\mathrm{R}+}\left(\varepsilon_{\downarrow}\right)+I_{2,\mathrm{R}+}\left(\varepsilon_{\downarrow}\right)\right]\rho_{\mathrm{dot},1,00}^{(n)} \\
& +\frac{\mathrm{i}\Gamma_{\mathrm{L}\uparrow}}{2\pi}\left[I_{1,\mathrm{L}-}\left(\varepsilon_{\uparrow}\right)+I_{2,\mathrm{L}-}\left(\varepsilon_{\uparrow}\right)\right]\rho_{\mathrm{dot},1,\uparrow\uparrow}^{(n)} \\
& +\frac{\mathrm{i}\Gamma_{\mathrm{R}\uparrow}}{2\pi}\left[I_{1,\mathrm{R}-}\left(\varepsilon_{\uparrow}\right)+I_{2,\mathrm{R}-}\left(\varepsilon_{\uparrow}\right)\right]\rho_{\mathrm{dot},1,\uparrow\uparrow}^{(n-1)} \\
& +\frac{\mathrm{i}\Gamma_{\mathrm{L}\downarrow}}{2\pi}\left[I_{1,\mathrm{L}-}\left(\varepsilon_{\downarrow}\right)+I_{2,\mathrm{L}-}\left(\varepsilon_{\downarrow}\right)\right]\rho_{\mathrm{dot},1,\downarrow\downarrow}^{(n)} \\
& +\frac{\mathrm{i}\Gamma_{\mathrm{R}\downarrow}}{2\pi}\left[I_{1,\mathrm{R}-}\left(\varepsilon_{\downarrow}\right)+I_{2,\mathrm{R}-}\left(\varepsilon_{\downarrow}\right)\right]\rho_{\mathrm{dot},1,\downarrow\downarrow}^{(n-1)},
\end{aligned} \tag{5.21}$$

其中

$$I_{1,\alpha+}\left(\Delta\right)=\int\mathrm{d}\omega\frac{g_{\alpha}\left(\omega\right)f_{\alpha}\left(\omega\right)}{\mathrm{i}\eta+\omega-\Delta}, \tag{5.22}$$

$$I_{1,\alpha-}\left(\Delta\right)=\int\mathrm{d}\omega\frac{g_{\alpha}\left(\omega\right)\left[1-f_{\alpha}\left(\omega\right)\right]}{\mathrm{i}\eta+\omega-\Delta}, \tag{5.23}$$

$$I_{2,\alpha+}\left(\Delta\right)=\int\mathrm{d}\omega\frac{g_{\alpha}\left(\omega\right)f_{\alpha}\left(\omega\right)}{\mathrm{i}\eta-\omega+\Delta}, \tag{5.24}$$

$$I_{2,\alpha-}\left(\Delta\right)=\int\mathrm{d}\omega\frac{g_{\alpha}\left(\omega\right)\left[1-f_{\alpha}\left(\omega\right)\right]}{\mathrm{i}\eta-\omega+\Delta}. \tag{5.25}$$

同理可得, $\dot{\rho}_{\mathrm{dot},1,\uparrow\uparrow}^{(n)}$、$\dot{\rho}_{\mathrm{dot},1,\downarrow\downarrow}^{(n)}$ 以及 $\dot{\rho}_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}^{(n)}$, 见附录 H. 然后, 根据第 3 章的电子计数统计方法, 可以计算电子通过单量子点的前四阶电流累积矩.

### 5.2.3 单量子点的电子计数统计性质

在本节的数值计算中, 单量子点的系统参数选取为 $\varepsilon_{\uparrow}=\varepsilon_{\downarrow}=1$, $U=5$, $p=p_{\mathrm{L}}=p_{\mathrm{R}}$, $k_{\mathrm{B}}T=0.04$, 其中能量 $U$ 单位为 meV. 对于量子点与左右电极的不对称隧穿耦合情形, 即 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}$ 为不同数值时, 在图 5.2 中, 给出了单量子点的电流前四阶累积矩随偏置电压的变化. 由图 5.2 可知, 非马尔可夫效应对单能级单量子点的电流前四阶累积矩没有影响, 即非马尔可夫效应消失, 马尔可夫效应起主要作用. 通

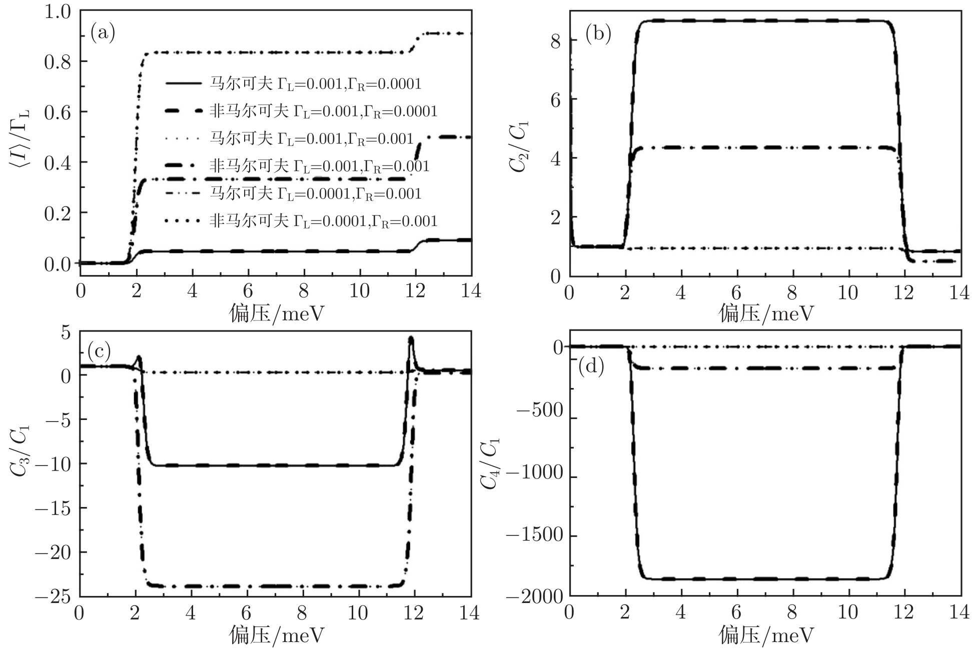


图 5.2 对于量子点与左右电极的不对称隧穿耦合情形, 单量子点的电流前四阶累积矩, 即 (a) 平均电流 ($\langle I\rangle$)、(b) 散粒噪声 ($C_2/C_1$)、(c) 偏斜度 ($C_3/C_1$)、(d) 峭度 ($C_4/C_1$) 随偏压的变化, 其中 $C_i$ 为电流的第 $i$ 阶零频累积矩

过计算和整理单量子点约化密度矩阵的矩阵元运动方程, 可以发现, 对于约化密度矩阵的矩阵元无非对角项的情形, 考虑非马尔可夫效应的矩阵元运动方程等价于马尔可夫情形.

下面, 给出 $\dot{\rho}^{(n)}_{\mathrm{dot},1,00}$、$\dot{\rho}^{(n)}_{\mathrm{dot},1,\uparrow\uparrow}$、$\dot{\rho}^{(n)}_{\mathrm{dot},1,\downarrow\downarrow}$ 以及 $\dot{\rho}^{(n)}_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}$ 四个矩阵元简化后的具体形式. 由附录 A 的式 (A.35)、(A.42)、(A.58)、(A.62) 可知

$$I_{1,\alpha+}(\Delta)=\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{\Delta-\mu_\alpha}{2\pi k_{\mathrm{B}}T}\right)-\ln\frac{W}{2\pi k_{\mathrm{B}}T}-\mathrm{i}\pi f^{(+)}_\alpha(\Delta), \tag{5.26}$$

$$I_{1,\alpha-}(\Delta)=-\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{\Delta-\mu_\alpha}{2\pi k_{\mathrm{B}}T}\right)+\ln\frac{W}{2\pi k_{\mathrm{B}}T}-\mathrm{i}\pi f^{(-)}_\alpha(\Delta), \tag{5.27}$$

$$I_{2,\alpha+}(\Delta)=-\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{\Delta-\mu_\alpha}{2\pi k_{\mathrm{B}}T}\right)+\ln\frac{W}{2\pi k_{\mathrm{B}}T}-\mathrm{i}\pi f^{(+)}_\alpha(\Delta), \tag{5.28}$$

$$I_{2,\alpha-}(\Delta)=\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{\Delta-\mu_\alpha}{2\pi k_{\mathrm{B}}T}\right)-\ln\frac{W}{2\pi k_{\mathrm{B}}T}-\mathrm{i}\pi f^{(-)}_\alpha(\Delta), \tag{5.29}$$

利用上面四式可得

$$I_{1,\alpha+}(\Delta)+I_{2,\alpha+}(\Delta)=-\mathrm{i}2\pi f_{\alpha}^{(+)}(\Delta), \tag{5.30}$$

$$I_{1,\alpha-}(\Delta)+I_{2,\alpha-}(\Delta)=-\mathrm{i}2\pi f_{\alpha}^{(-)}(\Delta). \tag{5.31}$$

将上面的式 (5.30) 和式 (5.31) 代入式 (5.21) 可得

$$\begin{aligned}
&\dot{\rho}_{\mathrm{dot},1,00}^{(n)}\\
=&-\left[\Gamma_{\mathrm{L}\uparrow}f_{\mathrm{L}}^{(+)}(\varepsilon_{\uparrow})+\Gamma_{\mathrm{R}\uparrow}f_{\mathrm{R}}^{(+)}(\varepsilon_{\uparrow})+\Gamma_{\mathrm{L}\downarrow}f_{\mathrm{L}}^{(+)}(\varepsilon_{\downarrow})+\Gamma_{\mathrm{R}\downarrow}f_{\mathrm{L}}^{(+)}(\varepsilon_{\downarrow})\right]\rho_{\mathrm{dot},1,00}^{(n)}\\
&+\Gamma_{\mathrm{L}\uparrow}f_{\mathrm{L}}^{(-)}(\varepsilon_{\uparrow})\rho_{\mathrm{dot},1,\uparrow\uparrow}^{(n)}+\Gamma_{\mathrm{R}\uparrow}f_{\mathrm{R}}^{(-)}(\varepsilon_{\uparrow})\rho_{\mathrm{dot},1,\uparrow\uparrow}^{(n-1)}\\
&+\Gamma_{\mathrm{L}\downarrow}f_{\mathrm{L}}^{(-)}(\varepsilon_{\downarrow})\rho_{\mathrm{dot},1,\downarrow\downarrow}^{(n)}+\Gamma_{\mathrm{R}\downarrow}f_{\mathrm{R}}^{(-)}(\varepsilon_{\downarrow})\rho_{\mathrm{dot},1,\downarrow\downarrow}^{(n-1)},
\end{aligned}\tag{5.32}$$

同理, 根据附录 H 的结果, 可得

$$\begin{aligned}
&\dot{\rho}_{\mathrm{dot},1,\uparrow\uparrow}^{(n)}\\
=&\Gamma_{\mathrm{L}\uparrow}f_{\mathrm{L}}^{(+)}(\varepsilon_{\uparrow})\rho_{\mathrm{dot},1,00}^{(n)}+\Gamma_{\mathrm{R}\uparrow}f_{\mathrm{R}}^{(+)}(\varepsilon_{\uparrow})\rho_{\mathrm{dot},1,00}^{(n+1)}\\
&-\left[\Gamma_{\mathrm{L}\uparrow}f_{\mathrm{L}}^{(-)}(\varepsilon_{\uparrow})+\Gamma_{\mathrm{R}\uparrow}f_{\mathrm{R}}^{(-)}(\varepsilon_{\uparrow})\right]\rho_{\mathrm{dot},1,\uparrow\uparrow}^{(n)}\\
&-\left[\Gamma_{\mathrm{L}\downarrow}f_{\mathrm{L}}^{(+)}(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow})+\Gamma_{\mathrm{R}\downarrow}f_{\mathrm{R}}^{(+)}(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow})\right]\rho_{\mathrm{dot},1,\uparrow\uparrow}^{(n)}\\
&+\Gamma_{\mathrm{L}\downarrow}f_{\mathrm{L}}^{(-)}(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow})\rho_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}^{(n)}+\Gamma_{\mathrm{R}\downarrow}f_{\mathrm{R}}^{(-)}(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow})\rho_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}^{(n-1)},
\end{aligned}\tag{5.33}$$

$$\begin{aligned}
&\dot{\rho}_{\mathrm{dot},1,\downarrow\downarrow}^{(n)}\\
=&\Gamma_{\mathrm{L}\downarrow}f_{\mathrm{L}}^{(+)}(\varepsilon_{\downarrow})\rho_{\mathrm{dot},1,00}^{(n)}+\Gamma_{\mathrm{R}\downarrow}f_{\mathrm{R}}^{(+)}(\varepsilon_{\downarrow})\rho_{\mathrm{dot},1,00}^{(n+1)}\\
&-\left[\Gamma_{\mathrm{L}\downarrow}f_{\mathrm{L}}^{(-)}(\varepsilon_{\downarrow})+\Gamma_{\mathrm{R}\downarrow}f_{\mathrm{R}}^{(-)}(\varepsilon_{\downarrow})\right]\rho_{\mathrm{dot},1,\downarrow\downarrow}^{(n)}\\
&-\left[\Gamma_{\mathrm{L}\uparrow}f_{\mathrm{L}}^{(+)}(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow})+\Gamma_{\mathrm{R}\uparrow}f_{\mathrm{R}}^{(+)}(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow})\right]\rho_{\mathrm{dot},1,\downarrow\downarrow}^{(n)}\\
&+\Gamma_{\mathrm{L}\uparrow}f_{\mathrm{L}}^{(-)}(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow})\rho_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}^{(n)}+\Gamma_{\mathrm{R}\uparrow}f_{\mathrm{R}}^{(-)}(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow})\rho_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}^{(n-1)},
\end{aligned}\tag{5.34}$$

$$\begin{aligned}
&\dot{\rho}_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}^{(n)}\\
=&\Gamma_{\mathrm{L}\downarrow}f_{\mathrm{L}}^{(+)}(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow})\rho_{\mathrm{dot},1,\uparrow\uparrow}^{(n)}+\Gamma_{\mathrm{R}\downarrow}f_{\mathrm{R}}^{(+)}(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow})\rho_{\mathrm{dot},1,\uparrow\uparrow}^{(n+1)}\\
&+\Gamma_{\mathrm{L}\uparrow}f_{\mathrm{L}}^{(+)}(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow})\rho_{\mathrm{dot},1,\downarrow\downarrow}^{(n)}+\Gamma_{\mathrm{R}\uparrow}f_{\mathrm{R}}^{(+)}(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow})\rho_{\mathrm{dot},1,\downarrow\downarrow}^{(n+1)}
\end{aligned}$$

$$
\begin{aligned}
&- \left[\Gamma_{\mathrm{L}\uparrow} f_{\mathrm{L}}^{(-)}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow}\right)+\Gamma_{\mathrm{R}\uparrow} f_{\mathrm{R}}^{(-)}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow}\right)\right] \rho_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}^{(n)} \\
&- \left[\Gamma_{\mathrm{L}\downarrow} f_{\mathrm{L}}^{(-)}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow}\right)+\Gamma_{\mathrm{R}\downarrow} f_{\mathrm{R}}^{(-)}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow}\right)\right] \rho_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}^{(n)},
\end{aligned} \tag{5.35}
$$

可以验证上面四式的结果与基于忽略电子库谱函数虚部的马尔可夫粒子数分辨量子主方程的数值结果相同.

在密度矩阵理论中, 约化密度矩阵的非对角元表征了量子系统的量子相干性, 因此, 由上面的计算可知, 非马尔可夫效应对量子点系统电子计数统计的影响可能联系到该系统的量子相干性. 为了进一步确认此结论, 下面以量子相干性可调的串联耦合双量子点和 T 型双量子点为例, 进一步验证上面的结论正确与否.

## 5.3 量子相干性可调的串联耦合双量子点

对于耦合双量子点, 根据其与源极 (左电极) 和漏极 (右电极) 的耦合方式, 分为三种情况: 串联耦合双量子点, 如图 5.1(b); T 型双量子点, 如图 5.1(c); 并联耦合双量子点. 这里, 讨论串联耦合双量子点和 T 型双量子点两种情况.

### 5.3.1 开放串联耦合双量子点系统的哈密顿量

一个串联耦合双量子点与两个电极耦合的开放量子系统的哈密顿量可以表示为

$$
H = H_{\mathrm{dot},2} + H_{\mathrm{leads},2} + H_{\mathrm{tun},2}, \tag{5.36}
$$

为方便讨论和简化计算, 忽略电子的自旋自由度, 此时, 式 (5.36) 中的第一项, 即串联耦合双量子点的哈密顿量可以表示为

$$
H_{\mathrm{dot},2} = \varepsilon_1 d_1^\dagger d_1 + \varepsilon_2 d_2^\dagger d_2 + U d_1^\dagger d_1 d_2^\dagger d_2 - J\left(d_1^\dagger d_2 + d_2^\dagger d_1\right), \tag{5.37}
$$

其中, $d_i^\dagger\,(d_i)$ 表示在第 $i$ 个量子点内的能级 $\varepsilon_i$ 上产生 (湮灭) 一个电子, $U$ 表示在不同量子点内两个电子之间的库仑相互作用. 但是, 在单个量子点内, 两个电子之间的库仑相互作用为无穷大, 即一个量子点内只能占据一个电子. 式 (5.37) 中的第四项为两个量子点之间的跳跃隧穿耦合项, 其强度用 $J$ 表示. 另外, 同样假设两个电极的电子弛豫过程足够快, 则其电子分布可以用平衡态的费米分布函数描述, 因而, 两个电极的哈密顿量可以表示为

$$
H_{\mathrm{leads},2} = \sum_{\alpha \boldsymbol{k}} \varepsilon_{\alpha \boldsymbol{k}} a_{\alpha \boldsymbol{k}}^\dagger a_{\alpha \boldsymbol{k}}, \tag{5.38}
$$

其中, $a_{\alpha\boldsymbol{k}}^\dagger\,(a_{\alpha\boldsymbol{k}})$ 表示在 $\alpha(\alpha=\mathrm{L},\mathrm{R})$ 电极上产生 (湮灭) 一个能量为 $\varepsilon_{\alpha\boldsymbol{k}}$、动量为 $\boldsymbol{k}$ 的电子. 相应地, 串联耦合双量子点与左右电极的隧穿耦合, 即式 (5.36) 中的第三项 $H_{\mathrm{tun},2}$ 可表示为

$$H_{\text{tun},2} = t_{\text{L}\boldsymbol{k}} a_{\text{L}\boldsymbol{k}}^{\dagger} d_1 + t_{\text{R}\boldsymbol{k}} a_{\text{R}\boldsymbol{k}}^{\dagger} d_2 + \text{H.c.} \tag{5.39}$$

### 5.3.2 耦合双量子点的本征值和本征态

对于式 (5.37) 描述的耦合双量子点, 其可能的电子状态可以用两个量子点内的电子数描述, 即,

$$|0,0\rangle = |0\rangle_1 |0\rangle_2, \quad \langle 0,0| = \langle 0|_2 \langle 0|_1, \tag{5.40}$$

$$|1,0\rangle = |1\rangle_1 |0\rangle_2, \quad \langle 0,1| = \langle 0|_2 \langle 1|_1, \tag{5.41}$$

$$|0,1\rangle = |0\rangle_1 |1\rangle_2, \quad \langle 1,0| = \langle 1|_2 \langle 0|_1, \tag{5.42}$$

$$|1,1\rangle = |1\rangle_1 |1\rangle_2, \quad \langle 1,1| = \langle 1|_2 \langle 1|_1, \tag{5.43}$$

上面四式可以组成对角化耦合双量子点哈密顿量的完备基. 首先, 将耦合双量子点的哈密顿量, 即式 (5.37), 作用到其空占据态, 即式 (5.40), 和双电子占据态, 即式 (5.43), 可得

$$H_{\text{dot},2} |0,0\rangle = \varepsilon_0 |0,0\rangle, \quad \varepsilon_0 = 0, \tag{5.44}$$

$$H_{\text{dot},2} |1,1\rangle = \varepsilon_{1,1} |1,1\rangle, \quad \varepsilon_{1,1} = \varepsilon_1 + \varepsilon_2 + U, \tag{5.45}$$

由式 (5.44) 和式 (5.45) 可知, 空占据态和双电子占据态本身即为耦合双量子点的本征态. 对于单电子占据态的情形, 将耦合双量子点的哈密顿量作用到两个单电子占据态, 即式 (5.41) 和式 (5.42), 可得

$$H_{\text{dot},2} |1,0\rangle = \varepsilon_1 |1,0\rangle - J |0,1\rangle, \tag{5.46}$$

$$H_{\text{dot},2} |0,1\rangle = -J |1,0\rangle + \varepsilon_2 |0,1\rangle, \tag{5.47}$$

由式 (5.46) 和式 (5.47) 可知, 两个单电子占据态 $|1,0\rangle$ 和 $|0,1\rangle$ 均不是耦合双量子点的本征态. 为了求单电子占据态情形下耦合双量子点的本征态, 将式 (5.46) 和式 (5.47) 写成如下的矩阵形式:

$$H_{\text{dot},2} \begin{pmatrix} |1,0\rangle \\ |0,1\rangle \end{pmatrix} = \begin{pmatrix} \varepsilon_1 & -J \\ -J & \varepsilon_2 \end{pmatrix} \begin{pmatrix} |1,0\rangle \\ |0,1\rangle \end{pmatrix} = M \begin{pmatrix} |1,0\rangle \\ |0,1\rangle \end{pmatrix}, \tag{5.48}$$

其中

$$M = \begin{pmatrix} \varepsilon_1 & -J \\ -J & \varepsilon_2 \end{pmatrix}. \tag{5.49}$$

此时, 求解耦合双量子点单电子占据态的本征态就转变为求式 (5.49) 的矩阵 $M$ 的本征值和本征态. 通过计算可得, 耦合双量子点单电子占据态的本征态和本征值可表示为

$$H_{\text{dot},2} |1\rangle^{\pm} = \varepsilon_{\pm} |1\rangle^{\pm}, \quad |1\rangle^{\pm} = a_{\pm} |1,0\rangle + b_{\pm} |0,1\rangle, \tag{5.50}$$

其中

$$\varepsilon_{\pm}=\frac{\varepsilon_1+\varepsilon_2\pm\sqrt{\left(\varepsilon_1-\varepsilon_2\right)^2+4J^2}}{2}, \tag{5.51}$$

$$a_{\pm}=\frac{\mp J}{\sqrt{\left(\varepsilon_{\pm}-\varepsilon_1\right)^2+J^2}}, \tag{5.52}$$

$$b_{\pm}=\frac{\pm\left(\varepsilon_{\pm}-\varepsilon_1\right)}{\sqrt{\left(\varepsilon_{\pm}-\varepsilon_1\right)^2+J^2}}. \tag{5.53}$$

此外, 两个非本征态的单电子占据态 $|1,0\rangle$ 和 $|0,1\rangle$ 可以用相应的本征态表示为

$$|1,0\rangle=a_{+}\left|1\right\rangle^{+}+a_{-}\left|1\right\rangle^{-}, \tag{5.54}$$

$$|0,1\rangle=b_{+}\left|1\right\rangle^{+}+b_{-}\left|1\right\rangle^{-}. \tag{5.55}$$

### 5.3.3 串联耦合双量子点的时间局域量子主方程

当串联耦合双量子点与源极、漏极之间的隧穿耦合强度为弱耦合时, 电子的顺序隧穿占主要地位, 相应地, 串联耦合双量子点约化密度矩阵的时间局域的粒子数分辨量子主方程可以表示为

$$\begin{aligned}
&\frac{\mathrm{d}\rho_{\mathrm{dot},2}^{(n)}}{\mathrm{d}t}\\
=&-\mathrm{i}\left[H_{\mathrm{dot},2},\rho_{\mathrm{dot},2}^{(n)}\right]-\Big[d_1^{\dagger}A_{\mathrm{L}}^{(-)}\left(L_{\mathrm{dot},2}\right)\rho_{\mathrm{dot},1}^{(n)}+d_2^{\dagger}A_{\mathrm{R}}^{(-)}\left(L_{\mathrm{dot},2}\right)\rho_{\mathrm{dot},2}^{(n)}\\
&+\rho_{\mathrm{dot},2}^{(n)}A_{\mathrm{L}}^{(+)}\left(L_{\mathrm{dot},2}\right)d_1^{\dagger}+\rho_{\mathrm{dot},2}^{(n)}A_{\mathrm{R}}^{(+)}\left(L_{\mathrm{dot},2}\right)d_2^{\dagger}-d_1^{\dagger}\rho_{\mathrm{dot},2}^{(n)}A_{\mathrm{L}}^{(+)}\left(L_{\mathrm{dot},2}\right)\\
&-d_2^{\dagger}\rho_{\mathrm{dot},2}^{(n+1)}A_{\mathrm{R}}^{(+)}\left(L_{\mathrm{dot},2}\right)-A_{\mathrm{L}}^{(-)}\left(L_{\mathrm{dot},2}\right)\rho_{\mathrm{dot},2}^{(n)}d_1^{\dagger}\\
&-A_{\mathrm{R}}^{(-)}\left(L_{\mathrm{dot},2}\right)\rho_{\mathrm{dot},2}^{(n-1)}d_2^{\dagger}+\mathrm{H.c.}\Big],
\end{aligned} \tag{5.56}$$

其中, 超算符和隧穿概率 $\Gamma_\alpha$ 定义为

$$A_{\mathrm{L}}^{(\pm)}\left(L_{\mathrm{dot},2}\right)=\frac{\Gamma_{\mathrm{L}}}{2\pi}\int\mathrm{d}\omega\int_{-\infty}^{t}\mathrm{d}t_1g_{\mathrm{L}}\left(\omega\right)f_{\mathrm{L}}^{(\pm)}\left(\omega\right)\mathrm{e}^{-\mathrm{i}\left(\omega+L_{\mathrm{dot},2}\right)\left(t-t_1\right)}d_1, \tag{5.57}$$

$$A_{\mathrm{R}}^{(\pm)}\left(L_{\mathrm{dot},2}\right)=\frac{\Gamma_{\mathrm{R}}}{2\pi}\int\mathrm{d}\omega\int_{-\infty}^{t}\mathrm{d}t_1g_{\mathrm{R}}\left(\omega\right)f_{\mathrm{R}}^{(\pm)}\left(\omega\right)\mathrm{e}^{-\mathrm{i}\left(\omega+L_{\mathrm{dot},2}\right)\left(t-t_1\right)}d_2, \tag{5.58}$$

$$\Gamma_\alpha=2\pi g_\alpha\left|t_\alpha\right|^2. \tag{5.59}$$

为计算串联耦合双量子点约化密度矩阵的矩阵元运动方程, 选取其四个本征态: $|0,0\rangle$, $|1\rangle^{+}$, $|1\rangle^{-}$, $|1,1\rangle$ 为完备基, 相应的矩阵元有如下六个:

$$\rho_{\mathrm{dot},2,00}^{(n)}=\langle 0,0|\,\rho_{\mathrm{dot},2}^{(n)}\,|0,0\rangle\,, \tag{5.60}$$

$$\rho_{\mathrm{dot},2,++}^{(n)}=\langle 1|^{+}\,\rho_{\mathrm{dot},2}^{(n)}\,|1\rangle^{+}\,, \tag{5.61}$$

$$\rho_{\mathrm{dot},2,+-}^{(n)}=\langle 1|^{+}\,\rho_{\mathrm{dot},2}^{(n)}\,|1\rangle^{-}\,, \tag{5.62}$$

$$\rho_{\mathrm{dot},2,-+}^{(n)}=\langle 1|^{-}\,\rho_{\mathrm{dot},2}^{(n)}\,|1\rangle^{+}\,, \tag{5.63}$$

$$\rho_{\mathrm{dot},2,--}^{(n)}=\langle 1|^{-}\,\rho_{\mathrm{dot},2}^{(n)}\,|1\rangle^{-}\,, \tag{5.64}$$

$$\rho_{\mathrm{dot},2,11,11}^{(n)}=\langle 1,1|\,\rho_{\mathrm{dot},2}^{(n)}\,|1,1\rangle\,. \tag{5.65}$$

下面计算矩阵元 $\rho_{\mathrm{dot},2,00}^{(n)}$ 的运动方程. 由式 (5.56) 可知

$$\begin{aligned}
&\dot{\rho}_{\mathrm{dot},2,00}^{(n)}\\
=&-\langle 0,0|\,\rho_{\mathrm{dot},2}^{(n)}A_{\mathrm{L}}^{(+)}\left(L_{\mathrm{dot},2}\right)d_1^{\dagger}\,|0,0\rangle-\langle 0,0|\,\rho_{\mathrm{dot},2}^{(n)}A_{\mathrm{R}}^{(+)}\left(L_{\mathrm{dot},2}\right)d_2^{\dagger}\,|0,0\rangle\\
&+\langle 0,0|\,A_{\mathrm{L}}^{(-)}\left(L_{\mathrm{dot},2}\right)\rho_{\mathrm{dot},2}^{(n)}d_1^{\dagger}\,|0,0\rangle+\langle 0,0|\,A_{\mathrm{R}}^{(-)}\left(L_{\mathrm{dot},2}\right)\rho_{\mathrm{dot},2}^{(n-1)}d_2^{\dagger}\,|0,0\rangle\\
&-\langle 0,0|\,d_1\left[A_{\mathrm{L}}^{(+)}\left(L_{\mathrm{dot},2}\right)\right]^{\dagger}\rho_{\mathrm{dot},2}^{(n)}\,|0,0\rangle-\langle 0,0|\,d_2\left[A_{\mathrm{R}}^{(+)}\left(L_{\mathrm{dot},2}\right)\right]^{\dagger}\rho_{\mathrm{dot},2}^{(n)}\,|0,0\rangle\\
&+\langle 0,0|\,d_1\rho_{\mathrm{dot},2}^{(n)}\left[A_{\mathrm{L}}^{(-)}\left(L_{\mathrm{dot},2}\right)\right]^{\dagger}|0,0\rangle+\langle 0,0|\,d_2\rho_{\mathrm{dot},2}^{(n-1)}\left[A_{\mathrm{R}}^{(-)}\left(L_{\mathrm{dot},2}\right)\right]^{\dagger}|0,0\rangle\,,
\end{aligned} \tag{5.66}$$

由于

$$d_1^{\dagger}\,|0,0\rangle=|1,0\rangle=a_{+}\,|1\rangle^{+}+a_{-}\,|1\rangle^{-}\,, \tag{5.67}$$

$$d_2^{\dagger}\,|0,0\rangle=|0,1\rangle=b_{+}\,|1\rangle^{+}+b_{-}\,|1\rangle^{-}\,, \tag{5.68}$$

则式 (5.66) 可以进一步表示为

$$\begin{aligned}
&\left.\dot{\rho}_{\mathrm{dot},2,00}^{(n)}\right|_{01}\\
=&-a_{+}\,\langle 0,0|\,\rho_{\mathrm{dot},2}^{(n)}A_{\mathrm{L}}^{(+)}\left(L_{\mathrm{dot},2}\right)|1\rangle^{+}-b_{+}\,\langle 0,0|\,\rho_{\mathrm{dot},2}^{(n)}A_{\mathrm{R}}^{(+)}\left(L_{\mathrm{dot},2}\right)|1\rangle^{+}\\
&-a_{-}\,\langle 0,0|\,\rho_{\mathrm{dot},2}^{(n)}A_{\mathrm{L}}^{(+)}\left(L_{\mathrm{dot},2}\right)|1\rangle^{-}-b_{-}\,\langle 0,0|\,\rho_{\mathrm{dot},2}^{(n)}A_{\mathrm{R}}^{(+)}\left(L_{\mathrm{dot},2}\right)|1\rangle^{-}\\
&-a_{+}\,\langle 1|^{+}\left[A_{\mathrm{L}}^{(+)}\left(L_{\mathrm{dot},2}\right)\right]^{\dagger}\rho_{\mathrm{dot},2}^{(n)}\,|0,0\rangle-b_{+}\,\langle 1|^{+}\left[A_{\mathrm{R}}^{(+)}\left(L_{\mathrm{dot},2}\right)\right]^{\dagger}\rho_{\mathrm{dot},2}^{(n)}\,|0,0\rangle\\
&-a_{-}\,\langle 1|^{-}\left[A_{\mathrm{L}}^{(+)}\left(L_{\mathrm{dot},2}\right)\right]^{\dagger}\rho_{\mathrm{dot},2}^{(n)}\,|0,0\rangle-b_{-}\,\langle 1|^{-}\left[A_{\mathrm{R}}^{(+)}\left(L_{\mathrm{dot},2}\right)\right]^{\dagger}\rho_{\mathrm{dot},2}^{(n)}\,|0,0\rangle\,,
\end{aligned} \tag{5.69}$$

$$
\begin{aligned}
&\dot{\rho}_{\mathrm{dot},2,00}^{(n)}\Big|_{02} \\
=&+a_{+}\langle 0,0|\, A_{\mathrm{L}}^{(-)}\left(L_{\mathrm{dot},2}\right)\rho_{\mathrm{dot},2}^{(n)}\,|1\rangle^{+}+b_{+}\langle 0,0|\, A_{\mathrm{R}}^{(-)}\left(L_{\mathrm{dot},2}\right)\rho_{\mathrm{dot},2}^{(n-1)}\,|1\rangle^{+} \\
&+a_{-}\langle 0,0|\, A_{\mathrm{L}}^{(-)}\left(L_{\mathrm{dot},2}\right)\rho_{\mathrm{dot},2}^{(n)}\,|1\rangle^{-}+b_{-}\langle 0,0|\, A_{\mathrm{R}}^{(-)}\left(L_{\mathrm{dot},2}\right)\rho_{\mathrm{dot},2}^{(n-1)}\,|1\rangle^{-} \\
&+a_{+}\langle 1|^{+}\,\rho_{\mathrm{dot},2}^{(n)}\left[A_{\mathrm{L}}^{(-)}\left(L_{\mathrm{dot},2}\right)\right]^{\dagger}|0,0\rangle+b_{+}\langle 1|^{+}\,\rho_{\mathrm{dot},2}^{(n-1)}\left[A_{\mathrm{R}}^{(-)}\left(L_{\mathrm{dot},2}\right)\right]^{\dagger}|0,0\rangle \\
&+a_{-}\langle 1|^{-}\,\rho_{\mathrm{dot},2}^{(n)}\left[A_{\mathrm{L}}^{(-)}\left(L_{\mathrm{dot},2}\right)\right]^{\dagger}|0,0\rangle+b_{-}\langle 1|^{-}\,\rho_{\mathrm{dot},2}^{(n-1)}\left[A_{\mathrm{R}}^{(-)}\left(L_{\mathrm{dot},2}\right)\right]^{\dagger}|0,0\rangle, \quad (5.70)
\end{aligned}
$$

为了计算式 (5.69) 和 (5.70), 需要对式 (5.57) 和 (5.58) 求关于时间 $t_1$ 的积分, 其结果可表示为

$$A_{\mathrm{L}}^{(\pm)}\left(L_{\mathrm{dot},2}\right)=\frac{\mathrm{i}\Gamma_{\mathrm{L}}}{2\pi}\int \mathrm{d}\omega\frac{g_{\mathrm{L}}\left(\omega\right)f_{\mathrm{L}}^{(\pm)}\left(\omega\right)}{\mathrm{i}\eta-\omega-L_{\mathrm{dot},2}}d_1, \quad (5.71)$$

$$A_{\mathrm{R}}^{(\pm)}\left(L_{\mathrm{dot},2}\right)=\frac{\mathrm{i}\Gamma_{\mathrm{R}}}{2\pi}\int \mathrm{d}\omega\frac{g_{\mathrm{R}}\left(\omega\right)f_{\mathrm{R}}^{(\pm)}\left(\omega\right)}{\mathrm{i}\eta-\omega-L_{\mathrm{dot},2}}d_2, \quad (5.72)$$

$$\left[A_{\mathrm{L}}^{(\pm)}\left(L_{\mathrm{dot},2}\right)\right]^{\dagger}=\frac{\mathrm{i}\Gamma_{\mathrm{L}}}{2\pi}\int \mathrm{d}\omega\frac{g_{\mathrm{L}}\left(\omega\right)f_{\mathrm{L}}^{(\pm)}\left(\omega\right)}{\mathrm{i}\eta+\omega-L_{\mathrm{dot},2}}d_1^{\dagger}, \quad (5.73)$$

$$\left[A_{\mathrm{R}}^{(\pm)}\left(L_{\mathrm{dot},2}\right)\right]^{\dagger}=\frac{\mathrm{i}\Gamma_{\mathrm{R}}}{2\pi}\int \mathrm{d}\omega\frac{g_{\mathrm{R}}\left(\omega\right)f_{\mathrm{R}}^{(\pm)}\left(\omega\right)}{\mathrm{i}\eta+\omega-L_{\mathrm{dot},2}}d_2^{\dagger}, \quad (5.74)$$

将式 (5.71)~式 (5.74) 代入式 (5.69) 和 (5.70), 并利用式 (5.17)~ 式 (5.20), 可得

$$
\begin{aligned}
\dot{\rho}_{\mathrm{dot},2,00}^{(n)}\Big|_{01}=&-\frac{\mathrm{i}\Gamma_{\mathrm{L}}}{2\pi}\big\{a_{+}a_{+}\left[I_{1,\mathrm{L}+}\left(\varepsilon_{+}\right)+I_{2,\mathrm{L}+}\left(\varepsilon_{+}\right)\right] \\
&+a_{-}a_{-}\left[I_{1,\mathrm{L}+}\left(\varepsilon_{-}\right)+I_{2,\mathrm{L}+}\left(\varepsilon_{-}\right)\right]\big\}\rho_{\mathrm{dot},2,00}^{(n)} \\
&-\frac{\mathrm{i}\Gamma_{\mathrm{R}}}{2\pi}\big\{b_{+}b_{+}\left[I_{1,\mathrm{R}+}\left(\varepsilon_{+}\right)+I_{2,\mathrm{R}+}\left(\varepsilon_{+}\right)\right] \\
&+b_{-}b_{-}\left[I_{1,\mathrm{R}+}\left(\varepsilon_{-}\right)+I_{2,\mathrm{R}+}\left(\varepsilon_{-}\right)\right]\big\}\rho_{\mathrm{dot},2,00}^{(n)}, \quad (5.75)
\end{aligned}
$$

$$
\begin{aligned}
\dot{\rho}_{\mathrm{dot},2,00}^{(n)}\Big|_{02\text{-}01}=&a_{+}a_{+}\frac{\mathrm{i}\Gamma_{\mathrm{L}}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{+}\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},2,++}^{(n)} \\
&+b_{+}b_{+}\frac{\mathrm{i}\Gamma_{\mathrm{R}}}{2\pi}\left[I_{1,\mathrm{R}-}\left(\varepsilon_{+}\right)+I_{2,\mathrm{R}-}\left(\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},2,++}^{(n-1)}, \quad (5.76)
\end{aligned}
$$

$$
\begin{aligned}
\dot{\rho}_{\mathrm{dot},2,00}^{(n)}\Big|_{02\text{-}02}=&a_{+}a_{-}\frac{\mathrm{i}\Gamma_{\mathrm{L}}}{2\pi}\left[I_{1,\mathrm{L}-}\left(\varepsilon_{-}\right)+I_{2,\mathrm{L}-}\left(\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},2,+-}^{(n)} \\
&+b_{+}b_{-}\frac{\mathrm{i}\Gamma_{\mathrm{R}}}{2\pi}\left[I_{1,\mathrm{R}-}\left(\varepsilon_{-}\right)+I_{2,\mathrm{R}-}\left(\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},2,+-}^{(n-1)}, \quad (5.77)
\end{aligned}
$$

$$
\begin{aligned}
\left.\dot{\rho}_{\mathrm{dot},2,00}^{(n)}\right|_{02\text{-}03} =& a_+a_-\frac{\mathrm{i}\Gamma_{\mathrm{L}}}{2\pi}\left[I_{1,\mathrm{L}-}\left(\varepsilon_+\right)+I_{2,\mathrm{L}-}\left(\varepsilon_-\right)\right]\rho_{\mathrm{dot},2,-+}^{(n)} \\
&+b_+b_-\frac{\mathrm{i}\Gamma_{\mathrm{R}}}{2\pi}\left[I_{1,\mathrm{R}-}\left(\varepsilon_+\right)+I_{2,\mathrm{R}-}\left(\varepsilon_-\right)\right]\rho_{\mathrm{dot},2,-+}^{(n-1)},
\end{aligned}
\tag{5.78}
$$

$$
\begin{aligned}
\left.\dot{\rho}_{\mathrm{dot},2,00}^{(n)}\right|_{02\text{-}04} =& a_-a_-\frac{\mathrm{i}\Gamma_{\mathrm{L}}}{2\pi}\left[I_{1,\mathrm{L}-}\left(\varepsilon_-\right)+I_{2,\mathrm{L}-}\left(\varepsilon_-\right)\right]\rho_{\mathrm{dot},2,--}^{(n)} \\
&+b_-b_-\frac{\mathrm{i}\Gamma_{\mathrm{R}}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_-\right)+I_{1,\mathrm{R}-}\left(\varepsilon_-\right)\right]\rho_{\mathrm{dot},2,--}^{(n-1)}.
\end{aligned}
\tag{5.79}
$$

同理, 可得约化密度矩阵的矩阵元运动方程$\dot{\rho}_{\mathrm{dot},2,++}^{(n)}$、$\dot{\rho}_{\mathrm{dot},2,+-}^{(n)}$、$\dot{\rho}_{\mathrm{dot},2,-+}^{(n)}$、$\dot{\rho}_{\mathrm{dot},2,--}^{(n)}$以及 $\dot{\rho}_{\mathrm{dot},2,11,11}^{(n)}$, 其结果见附录 H.

### 5.3.4　串联耦合双量子点的电子计数统计性质

在耦合双量子点中, 电子的动力学过程主要取决于如下两个因素: ① 两个量子点之间的隧穿耦合强度 $J$; ② 两个量子点与源极、漏极的隧穿耦合强度 $\Gamma_{\mathrm{L}}$ 和 $\Gamma_{\mathrm{R}}$. 这里, 重点研究两个量子点之间的隧穿耦合强度 $J$ 可以强烈影响串联耦合双量子点内电子动力学特性的参数区域, 即 $J<(\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}})$, 此时, 该系统约化密度矩阵的非对角元在电子隧穿过程中起关键作用 [49-51]. 在下面的数值计算中, 串联耦合双量子点的系统参数选为: $\varepsilon_1=\varepsilon_2=1$, $J=0.001$, $U=4$ 和 $k_{\mathrm{B}}T=0.05$, 能量单位为 meV.

首先, 讨论量子点 2 与右电极 (漏极) 的隧穿耦合强度 $\Gamma_{\mathrm{R}}$ 大于量子点 1 与左电极 (源极) 的隧穿耦合强度 $\Gamma_{\mathrm{L}}$, 即 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}<1$ 的情形. 由图 5.3 可知, 当 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}=0.1$ 时, 即使量子点 2 与右电极 (漏极) 的隧穿耦合强度 $\Gamma_{\mathrm{R}}$ 大于两个量子点之间的隧穿耦合强度 $J$ 数倍, 非马尔可夫效应也仅对系统的电流前四阶累积矩有一个非常弱的影响, 且仅在高阶累积矩偏斜度和峭度上有微小的变化, 如图 5.3(c) 和图 5.3(d). 但是, 对于 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}\geqslant 1$ 的情形, 非马尔可夫效应对系统的电流前四阶累积矩有一个非常重要的影响, 见图 5.4 和图 5.5. 特别是, 当量子点 1 与左电极 (源极) 的隧穿耦合强度 $\Gamma_{\mathrm{L}}$ 大于两个量子点之间的隧穿耦合强度 $J$ 数倍, 即 $\Gamma_{\mathrm{L}}/J>1$, 且量子点 1 与左电极 (源极) 的隧穿耦合强度 $\Gamma_{\mathrm{L}}$ 大于量子点 2 与右电极 (漏极) 的隧穿耦合强度 $\Gamma_{\mathrm{R}}$ 时, 如 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}=10$, 非马尔可夫效应可以诱导一个强的负微分电导和超泊松噪声, 见图 5.5(a) 和 5.5(b). 另外, 在 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}\geqslant 1$ 和 $\Gamma_{\mathrm{L}}/J>1$ 的情形下, 电流的高阶累积矩偏斜度和峭度的数值可以发生从正值 (负值) 到负值 (正值) 的转变, 见图 5.4(c)、(d) 和图 5.5(d). 由统计理论可知, 偏斜度和峭度分别刻画了一段时间间隔 $t$ 内电子数在平均传输电子数目 $\bar{n}$ 附近分布的不对称性和其分布峰的峭度, 因而, 偏斜度和峭度的大小和正负可以提供超越散粒噪声的关于电子计数统计的进一步信息.

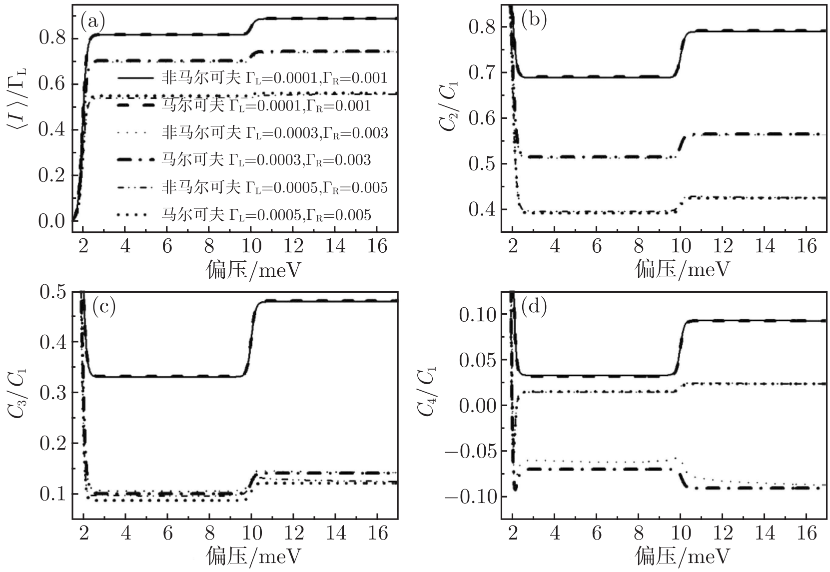


图 5.3 对于 $\Gamma_{\rm R}$ 为不同数值且 $\Gamma_{\rm L}/\Gamma_{\rm R}=0.1$ 的情形, 串联耦合双量子点的电流前四阶累积矩, 即 (a) 平均电流 ($\langle I\rangle$)、(b) 散粒噪声 ($C_2/C_1$)、(c) 偏斜度 ($C_3/C_1$)、(d) 峭度 ($C_4/C_1$) 随偏压的变化, 其中 $C_i$ 为电流的第 $i$ 阶零频累积矩

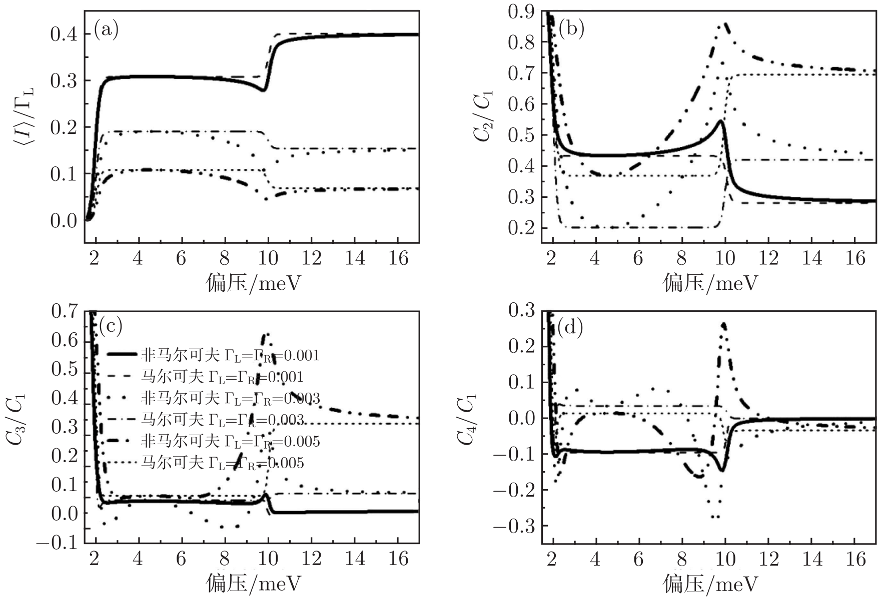


图 5.4 对于 $\Gamma_{\rm R}$ 为不同数值且 $\Gamma_{\rm L}/\Gamma_{\rm R}=1$ 情形, 串联耦合双量子点的电流前四阶累积矩, 即 (a) 平均电流 ($\langle I\rangle$)、(b) 散粒噪声 ($C_2/C_1$)、(c) 偏斜度 ($C_3/C_1$)、(d) 峭度 ($C_4/C_1$) 随偏压的变化, 其中 $C_i$ 为电流的第 $i$ 阶零频累积矩

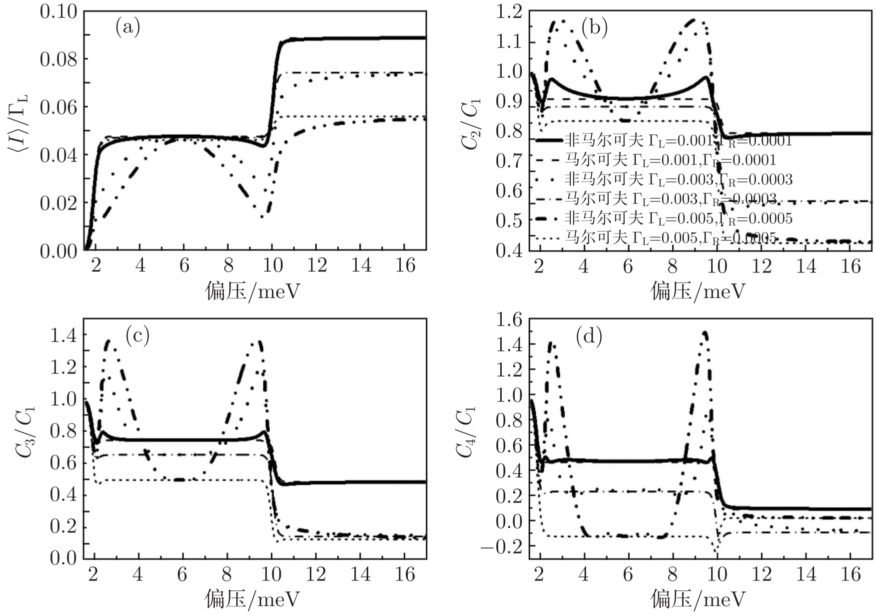


图 5.5　对于 $\Gamma_{\mathrm{R}}$ 为不同数值且 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}=10$ 情形, 串联耦合双量子点的电流前四阶累积矩, 即 (a) 平均电流 ($\langle I\rangle$)、(b) 散粒噪声 ($C_2/C_1$)、(c) 偏斜度 ($C_3/C_1$)、(d) 峭度 ($C_4/C_1$) 随偏压的变化, 其中 $C_i$ 为电流的第 $i$ 阶零频累积矩

为讨论电流噪声的物理机制, 对于上面选取的串联耦合双量子点参数, 两个单电子占据态的本征态和本征值可以表示为

$$|1\rangle^{\pm}=\mp\frac{\sqrt{2}}{2}\,|1,0\rangle+\frac{\sqrt{2}}{2}\,|0,1\rangle\,, \tag{5.80}$$

$$\varepsilon_{+}=\varepsilon_{-}=\varepsilon, \tag{5.81}$$

$$a_{\pm}=\mp\frac{\sqrt{2}}{2},\quad b_{\pm}=\frac{\sqrt{2}}{2}, \tag{5.82}$$

这里, 已经利用了关系式 $\varepsilon_1=\varepsilon_2=\varepsilon$ 和 $\varepsilon\gg J$. 此时, 根据式 (5.75)~ 式 (5.79) 和附录 H 的结果, 约化密度矩阵六个矩阵元的运动方程可以表示为

$$\begin{aligned}
&\dot{\rho}^{(n)}_{\mathrm{dot},2,00}\\
=&-\left[\Gamma_{\mathrm{L}}f^{(+)}_{\mathrm{L}}\left(\varepsilon\right)+\Gamma_{\mathrm{R}}f^{(+)}_{\mathrm{R}}\left(\varepsilon\right)\right]\rho^{(n)}_{\mathrm{dot},2,00}\\
&+\frac{\Gamma_{\mathrm{L}}}{2}f^{(-)}_{\mathrm{L}}\left(\varepsilon\right)\rho^{(n)}_{\mathrm{dot},2,++}+\frac{\Gamma_{\mathrm{R}}}{2}f^{(-)}_{\mathrm{R}}\left(\varepsilon\right)\rho^{(n-1)}_{\mathrm{dot},2,++}\\
&-\frac{\Gamma_{\mathrm{L}}}{2}f^{(-)}_{\mathrm{L}}\left(\varepsilon\right)\rho^{(n)}_{\mathrm{dot},2,+-}+\frac{\Gamma_{\mathrm{R}}}{2}f^{(-)}_{\mathrm{R}}\left(\varepsilon\right)\rho^{(n-1)}_{\mathrm{dot},2,+-}
\end{aligned}$$

$$
\begin{aligned}
&-\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(-)}(\varepsilon)\,\rho_{\mathrm{dot},2,-+}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(-)}(\varepsilon)\,\rho_{\mathrm{dot},2,-+}^{(n-1)}\\
&+\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(-)}(\varepsilon)\,\rho_{\mathrm{dot},2,--}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(-)}(\varepsilon)\,\rho_{\mathrm{dot},2,--}^{(n-1)},
\end{aligned}\tag{5.83}
$$

$$
\begin{aligned}
&\dot{\rho}_{\mathrm{dot},2,++}^{(n)}\\
=&\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(+)}(\varepsilon)\,\rho_{\mathrm{dot},2,00}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(+)}(\varepsilon)\,\rho_{\mathrm{dot},2,00}^{(n+1)}\\
&-\frac{1}{2}\left\{\Gamma_{\mathrm{L}}\left[f_{\mathrm{L}}^{(-)}(\varepsilon)+f_{\mathrm{L}}^{(+)}(\varepsilon+U)\right]+\Gamma_{\mathrm{R}}\left[f_{\mathrm{R}}^{(-)}(\varepsilon)+f_{\mathrm{R}}^{(+)}(\varepsilon+U)\right]\right\}\rho_{\mathrm{dot},2,++}^{(n)}\\
&+\frac{1}{4\pi}\left[\Gamma_{\mathrm{L}}\left(\mathrm{i}\phi_{\mathrm{L}}-\pi f_{\mathrm{L}}\right)-\Gamma_{\mathrm{R}}\left(\mathrm{i}\phi_{\mathrm{R}}-\pi f_{\mathrm{R}}\right)\right]\rho_{\mathrm{dot},2,+-}^{(n)}\\
&-\frac{1}{4\pi}\left\{\Gamma_{\mathrm{L}}\left(\mathrm{i}\phi_{\mathrm{L}}+\pi f_{\mathrm{L}}\right)\rho_{\mathrm{dot},2,-+}^{(n)}-\Gamma_{\mathrm{R}}\left(\mathrm{i}\phi_{\mathrm{R}}+\pi f_{\mathrm{R}}\right)\right\}\rho_{\mathrm{dot},2,-+}^{(n)}\\
&+\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(-)}(\varepsilon+U)\,\rho_{\mathrm{dot},2,11,11}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(-)}(\varepsilon+U)\,\rho_{\mathrm{dot},2,11,11}^{(n-1)},
\end{aligned}\tag{5.84}
$$

$$
\begin{aligned}
&\dot{\rho}_{\mathrm{dot},2,+-}^{(n)}\\
=&-\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(+)}(\varepsilon)\,\rho_{\mathrm{dot},2,00}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(+)}(\varepsilon)\,\rho_{\mathrm{dot},2,00}^{(n+1)}\\
&+\frac{1}{4\pi}\left[\Gamma_{\mathrm{L}}\left(\mathrm{i}\phi_{\mathrm{L}}-\pi f_{\mathrm{L}}\right)\rho_{\mathrm{dot},2,++}^{(n)}-\Gamma_{\mathrm{R}}\left(\mathrm{i}\phi_{\mathrm{R}}-\pi f_{\mathrm{R}}\right)\right]\rho_{\mathrm{dot},2,++}^{(n)}\\
&-2\mathrm{i}J\rho_{\mathrm{dot},2,+-}^{(n)}\\
&-\frac{1}{2}\left\{\Gamma_{\mathrm{L}}\left[f_{\mathrm{L}}^{(+)}(\varepsilon+U)+f_{\mathrm{L}}^{(-)}(\varepsilon)\right]+\Gamma_{\mathrm{R}}\left[f_{\mathrm{R}}^{(+)}(\varepsilon+U)+f_{\mathrm{R}}^{(-)}(\varepsilon)\right]\right\}\rho_{\mathrm{dot},2,+-}^{(n)}\\
&-\frac{1}{4\pi}\left[\Gamma_{\mathrm{L}}\left(\mathrm{i}\phi_{\mathrm{L}}+\pi f_{\mathrm{L}}\right)\rho_{\mathrm{dot},2,--}^{(n)}-\Gamma_{\mathrm{R}}\left(\mathrm{i}\phi_{\mathrm{R}}+\pi f_{\mathrm{R}}\right)\right]\rho_{\mathrm{dot},2,--}^{(n)}\\
&+\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(-)}(\varepsilon+U)\,\rho_{\mathrm{dot},2,11,11}^{(n)}-\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(-)}(\varepsilon+U)\,\rho_{\mathrm{dot},2,11,11}^{(n-1)},
\end{aligned}\tag{5.85}
$$

$$
\begin{aligned}
&\dot{\rho}_{\mathrm{dot},2,-+}^{(n)}\\
=&-\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(+)}(\varepsilon)\,\rho_{\mathrm{dot},2,00}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(+)}(\varepsilon)\,\rho_{\mathrm{dot},2,00}^{(n+1)}\\
&-\frac{1}{4\pi}\left[\Gamma_{\mathrm{L}}\left(\mathrm{i}\phi_{\mathrm{L}}+\pi f_{\mathrm{L}}\right)-\Gamma_{\mathrm{R}}\left(\mathrm{i}\phi_{\mathrm{R}}+\pi f_{\mathrm{R}}\right)\right]\rho_{\mathrm{dot},2,++}^{(n)}
\end{aligned}
$$

$$
\begin{aligned}
&+2\mathrm{i}J\rho_{\mathrm{dot},2,-+}^{(n)}\\
&-\frac{1}{2}\left\{\Gamma_{\mathrm{L}}\left[f_{\mathrm{L}}^{(+)}(\varepsilon+U)+f_{\mathrm{L}}^{(-)}(\varepsilon)\right]+\Gamma_{\mathrm{R}}\left[f_{\mathrm{R}}^{(+)}(\varepsilon+U)+f_{\mathrm{R}}^{(-)}(\varepsilon)\right]\right\}\rho_{\mathrm{dot},2,-+}^{(n)}\\
&+\frac{1}{4\pi}\left[\Gamma_{\mathrm{L}}(\mathrm{i}\phi_{\mathrm{L}}-\pi f_{\mathrm{L}})-\Gamma_{\mathrm{R}}(\mathrm{i}\phi_{\mathrm{R}}-\pi f_{\mathrm{R}})\right]\rho_{\mathrm{dot},2,--}^{(n)}\\
&+\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(-)}(\varepsilon+U)\rho_{\mathrm{dot},2,11,11}^{(n)}-\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(-)}(\varepsilon+U)\rho_{\mathrm{dot},2,11,11}^{(n-1)},
\end{aligned}\tag{5.86}
$$

$$
\begin{aligned}
&\dot{\rho}_{\mathrm{dot},2,--}^{(n)}\\
=&\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(+)}(\varepsilon)\rho_{\mathrm{dot},2,00}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(+)}(\varepsilon)\rho_{\mathrm{dot},2,00}^{(n+1)}\\
&-\frac{1}{4\pi}\left[\Gamma_{\mathrm{L}}(\mathrm{i}\phi_{\mathrm{L}}+\pi f_{\mathrm{L}})\rho_{\mathrm{dot},2,+-}^{(n)}-\Gamma_{\mathrm{R}}(\mathrm{i}\phi_{\mathrm{R}}+\pi f_{\mathrm{R}})\right]\rho_{\mathrm{dot},2,+-}^{(n)}\\
&+\frac{1}{4\pi}\left[\Gamma_{\mathrm{L}}(\mathrm{i}\phi_{\mathrm{L}}-\pi f_{\mathrm{L}})\rho_{\mathrm{dot},2,-+}^{(n)}-\Gamma_{\mathrm{R}}(\mathrm{i}\phi_{\mathrm{R}}-\pi f_{\mathrm{R}})\right]\rho_{\mathrm{dot},2,-+}^{(n)}\\
&-\frac{1}{2}\left\{\Gamma_{\mathrm{L}}\left[f_{\mathrm{L}}^{(+)}(\varepsilon+U)+f_{\mathrm{L}}^{(-)}(\varepsilon)\right]+\Gamma_{\mathrm{R}}\left[f_{\mathrm{R}}^{(+)}(\varepsilon+U)+f_{\mathrm{R}}^{(-)}(\varepsilon)\right]\right\}\rho_{\mathrm{dot},2,--}^{(n)}\\
&+\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(-)}(\varepsilon+U)\rho_{\mathrm{dot},2,11,11}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(-)}(\varepsilon+U)\rho_{\mathrm{dot},2,11,11}^{(n-1)},
\end{aligned}\tag{5.87}
$$

$$
\begin{aligned}
&\dot{\rho}_{\mathrm{dot},2,11,11}^{(n)}\\
=&\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(+)}(\varepsilon+U)\rho_{\mathrm{dot},2,++}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(+)}(\varepsilon+U)\rho_{\mathrm{dot},2,++}^{(n+1)}\\
&+\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(+)}(\varepsilon+U)\rho_{\mathrm{dot},2,+-}^{(n)}-\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(+)}(\varepsilon+U)\rho_{\mathrm{dot},2,+-}^{(n+1)}\\
&+\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(+)}(\varepsilon+U)\rho_{\mathrm{dot},2,-+}^{(n)}-\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(+)}(\varepsilon+U)\rho_{\mathrm{dot},2,-+}^{(n+1)}\\
&+\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(+)}(\varepsilon+U)\rho_{\mathrm{dot},2,--}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(+)}(\varepsilon+U)\rho_{\mathrm{dot},2,--}^{(n+1)}\\
&-\left[\Gamma_{\mathrm{L}}f_{\mathrm{L}}^{(-)}(\varepsilon+U)+\Gamma_{\mathrm{R}}f_{\mathrm{R}}^{(-)}(\varepsilon+U)\right]\rho_{\mathrm{dot},2,11,11}^{(n)},
\end{aligned}\tag{5.88}
$$

其中上面简化中用到了如下关系式:

$$
I_{2,\alpha+}(\varepsilon+U)-I_{1,\alpha-}(\varepsilon)=-\phi_{\alpha}-\mathrm{i}\pi f_{\alpha},\tag{5.89}
$$

$$
I_{1,\alpha+}(\varepsilon+U)-I_{2,\alpha-}(\varepsilon)=\phi_{\alpha}-\mathrm{i}\pi f_{\alpha},\tag{5.90}
$$

$$\phi_\alpha = \phi_\alpha(\varepsilon+U) - \phi_\alpha(\varepsilon), \tag{5.91}$$

$$f_\alpha = f_\alpha^{(+)}(\varepsilon+U) - f_\alpha^{(-)}(\varepsilon), \tag{5.92}$$

$$\phi_\alpha(\Delta) = \mathrm{Re}\Psi\left(\frac{1}{2} + \mathrm{i}\frac{\Delta-\mu_\alpha}{2\pi k_{\mathrm{B}}T}\right). \tag{5.93}$$

由式 (5.83)~式 (5.88) 可知, 与马尔可夫的情形相比, 非马尔可夫效应很明显由系统约化密度矩阵的非对角元, 即串联耦合双量子点的量子相干性体现. 由图 5.6(a) 可知, 函数 $\phi_{\mathrm{L}}-0.1\phi_{\mathrm{R}}$ 和 $\phi_{\mathrm{L}}-\phi_{\mathrm{R}}$ 随着偏压的增大呈现出一个非常明显的数值变化, 尤其是在有新的电子输运通道开始参与量子输运的偏压 $V_{\mathrm{b}}=2$ 和 $V_{\mathrm{b}}=10$ 附近; 但是, 随着偏压的增大, 函数 $0.1\phi_{\mathrm{L}}-\phi_{\mathrm{R}}$ 呈现出一个非常缓慢的数值变化. 因而, 与 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}\geqslant 1$ 的情形相对, 非马尔可夫效应在 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}\geqslant 1$ 情形下对串联耦合双量子点的电流高阶累积矩有一个更加明显的影响. 其相应的物理机制可以作如下理解: 当量子点 2 与右电极 (漏极) 的隧穿耦合强度 $\Gamma_{\mathrm{R}}$ 小于或者远小于两个量子点之间的隧穿耦合强度 $J$ 时, 从量子点 1 隧穿到量子点 2 的传导电子并不能很快地隧穿出量子点 2 达到漏极, 因此, 可以继续影响电子的动力学特性, 进而影响其电子计数统计特性.

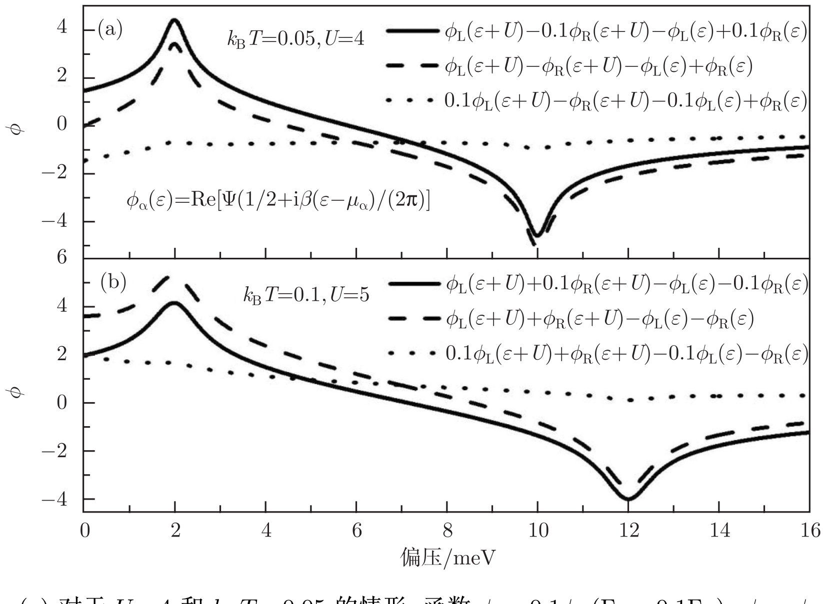


图 5.6 (a) 对于 $U=4$ 和 $k_{\mathrm{B}}T=0.05$ 的情形, 函数 $\phi_{\mathrm{L}}-0.1\phi_{\mathrm{R}}(\Gamma_{\mathrm{R}}=0.1\Gamma_{\mathrm{L}})$、$\phi_{\mathrm{L}}-\phi_{\mathrm{R}}(\Gamma_{\mathrm{R}}=\Gamma_{\mathrm{L}})$ 和 $0.1\phi_{\mathrm{L}}-\phi_{\mathrm{R}}(\Gamma_{\mathrm{L}}=0.1\Gamma_{\mathrm{R}})$ 随偏压的变化. (b) 对于 $U=5$ 和 $k_{\mathrm{B}}T=0.1$ 的情形, 函数 $\phi_{\mathrm{L}}+0.1\phi_{\mathrm{R}}(\Gamma_{\mathrm{R}}=0.1\Gamma_{\mathrm{L}})$、$\phi_{\mathrm{L}}+\phi_{\mathrm{R}}(\Gamma_{\mathrm{R}}=\Gamma_{\mathrm{L}})$ 和 $0.1\phi_{\mathrm{L}}+\phi_{\mathrm{R}}(\Gamma_{\mathrm{L}}=0.1\Gamma_{\mathrm{R}})$ 随偏压的变化

另外, 当两个量子点之间的隧穿耦合强度 $J$ 远大于两个量子点与源极、漏极的隧穿耦合强度 $\Gamma_{\mathrm{L}}$ 和 $\Gamma_{\mathrm{R}}$, 即 $J \gg (\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}})$ 时, 系统的量子相干性, 即系统的约化密度矩阵的非对角元对其电子隧穿过程影响非常弱或者几乎没有影响. 为了说明, 在系统量子相干性很弱时, 非马尔可夫效应对其电子计数统计影响也非常弱或者几乎没有影响, 在图 5.7 中, 给出了电流的前四阶累积矩在 $J=1$ 时在如下三种情形下随偏压的变化: ① 在马尔可夫情形下仅考虑约化密度矩阵的对角元; ② 在马尔可夫情形下考虑约化密度矩阵的非对角元; ③ 在非马尔可夫情形下考虑约化密度矩阵的非对角元. 由图 5.7 可知, 非马尔可夫效应在 $J \gg (\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}})$ 情形下确实对系统的电子计数统计几乎没有影响. 因此, 非马尔可夫效应对串联耦合双量子点电子计数统计特性的影响依赖于其量子相干性和量子点体系与源极、漏极的耦合强度. 为了证明这个结论是否普遍成立, 下一小节以 T 型双量子点为例进一步说明.

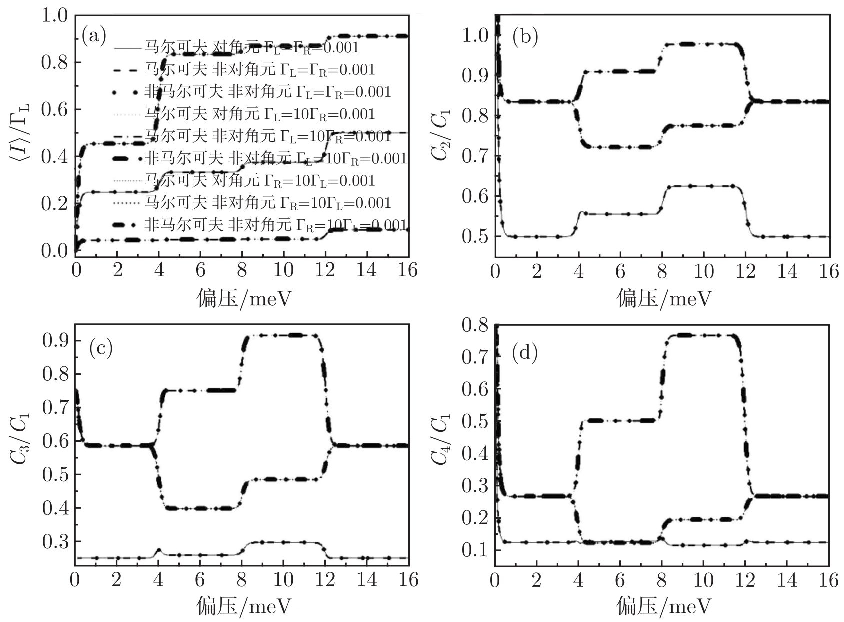


图 5.7 对于 $J=1$ 情形, 串联耦合双量子点的电流前四阶累积矩, 即 (a) 平均电流 ($\langle I\rangle$)、(b) 散粒噪声 ($C_2/C_1$)、(c) 偏斜度 ($C_3/C_1$)、(d) 峭度 ($C_4/C_1$) 随偏压的变化, 其中 $C_i$ 为电流的第 $i$ 阶零频累积矩

## 5.4 量子相干性可调的 T 型双量子点

在本节中, 继续研究非马尔可夫效应对 T 型双量子点电子计数统计特性的影响是否同样依赖于其量子相干性, 以验证 5.3 小节中的结论是否具有普遍性.

### 5.4.1 开放 T 型耦合双量子点系统的哈密顿量

对于 T 型双量子点, 与串联耦合双量子点相比, 除了仅有量子点 1 与源极和漏极两个电子库弱耦合外, 其余均相同, 即 $H_{\text{dot},3}=H_{\text{dot},2}$ 和 $H_{\text{leads},3}=H_{\text{leads},2}$. 此时, T 型双量子点与左右电极的隧穿耦合哈密顿量 $H_{\text{tun},3}$ 可表示为

$$H_{\text{tun},3}=t_{\mathrm{L}\boldsymbol{k}}a_{\mathrm{L}\boldsymbol{k}}^{\dagger}d_1+t_{\mathrm{R}\boldsymbol{k}}a_{\mathrm{R}\boldsymbol{k}}^{\dagger}d_1+\text{H.c.}. \tag{5.94}$$

### 5.4.2 T 型耦合双量子点的时间局域量子主方程

当串联耦合双量子点与源极、漏极之间的隧穿耦合强度为弱耦合时, 电子的顺序隧穿占主要地位, 相应地, 串联耦合双量子点约化密度矩阵的时间局域的粒子数分辨量子主方程可以表示为

$$\begin{aligned}
&\frac{\mathrm{d}\rho_{\text{dot},3}^{(n)}}{\mathrm{d}t}\\
=&-\mathrm{i}\left[H_{\text{dot},3},\rho_{\text{dot},3}^{(n)}\right]-\Big[d_1^{\dagger}A_{\mathrm{L}}^{(-)}\left(\mathrm{L}_{\text{dot},3}\right)\rho_{\text{dot},3}^{(n)}+d_1^{\dagger}A_{\mathrm{R}}^{(-)}\left(L_{\text{dot},3}\right)\rho_{\text{dot},3}^{(n)}\\
&+\rho_{\text{dot},3}^{(n)}A_{\mathrm{L}}^{(+)}\left(L_{\text{dot},3}\right)d_1^{\dagger}+\rho_{\text{dot},3}^{(n)}A_{\mathrm{R}}^{(+)}\left(L_{\text{dot},3}\right)d_1^{\dagger}-d_1^{\dagger}\rho_{\text{dot},3}^{(n)}A_{\mathrm{L}}^{(+)}\left(L_{\text{dot},3}\right)\\
&-d_1^{\dagger}\rho_{\text{dot},3}^{(n+1)}A_{\mathrm{R}}^{(+)}\left(L_{\text{dot},3}\right)-A_{\mathrm{L}}^{(-)}\left(L_{\text{dot},3}\right)\rho_{\text{dot},3}^{(n)}d_1^{\dagger}\\
&-A_{\mathrm{R}}^{(-)}\left(L_{\text{dot},3}\right)\rho_{\text{dot},3}^{(n-1)}d_1^{\dagger}+\text{H.c.}\Big],
\end{aligned} \tag{5.95}$$

其中, 超算符和隧穿概率 $\Gamma_\alpha$ 定义为

$$A_{\alpha}^{(\pm)}\left(L_{\text{dot},3}\right)=\frac{\Gamma_\alpha}{2\pi}\int\mathrm{d}\omega\int_{-\infty}^{t}\mathrm{d}t_1 g_\alpha\left(\omega\right)f_{\alpha}^{(\pm)}\left(\omega\right)\mathrm{e}^{-\mathrm{i}\left(\omega+L_{\text{dot},3}\right)\left(t-t_1\right)}d_1, \tag{5.96}$$

$$\Gamma_\alpha=2\pi g_\alpha\left|t_\alpha\right|^2. \tag{5.97}$$

同样, 为计算 T 型双量子点约化密度矩阵的矩阵元运动方程, 选取其四个本征态: $|0,0\rangle$, $|1\rangle^{+}$, $|1\rangle^{-}$, $|1,1\rangle$ 为完备基, 与串联耦合双量子点情形相同, 相应的矩阵元有如下六个:

$$\rho_{\text{dot},3,00}^{(n)}=\langle 0,0|\,\rho_{\text{dot},3}^{(n)}\,|0,0\rangle\,, \tag{5.98}$$

$$\rho_{\text{dot},3,++}^{(n)}=\langle 1|^{+}\,\rho_{\text{dot},3}^{(n)}\,|1\rangle^{+}\,, \tag{5.99}$$

$$\rho_{\text{dot},3,+-}^{(n)}=\langle 1|^{+}\,\rho_{\text{dot},3}^{(n)}\,|1\rangle^{-}\,, \tag{5.100}$$

$$\rho_{\text{dot},3,-+}^{(n)}=\langle 1|^{-}\,\rho_{\text{dot},3}^{(n)}\,|1\rangle^{+}\,, \tag{5.101}$$

$$\rho^{(n)}_{\mathrm{dot},3,--} = \langle 1|^{-}\, \rho^{(n)}_{\mathrm{dot},3}\, |1\rangle^{-}\,, \tag{5.102}$$

$$\rho^{(n)}_{\mathrm{dot},3,11,11} = \langle 1,1|\, \rho^{(n)}_{\mathrm{dot},3}\, |1,1\rangle\,. \tag{5.103}$$

下面计算矩阵元 $\rho^{(n)}_{\mathrm{dot},3,00}$ 的运动方程. 由式 (5.95) 可知

$$\begin{aligned}
\dot{\rho}^{(n)}_{\mathrm{dot},3,00} = & -\langle 0,0|\, \rho^{(n)}_{\mathrm{dot},3} A^{(+)}_{\mathrm{L}}\left(L_{\mathrm{dot},3}\right) d^{\dagger}_{1}\, |0,0\rangle \\
& -\langle 0,0|\, \rho^{(n)}_{\mathrm{dot},3} A^{(+)}_{\mathrm{R}}\left(L_{\mathrm{dot},3}\right) d^{\dagger}_{1}\, |0,0\rangle \\
& +\langle 0,0|\, A^{(-)}_{\mathrm{L}}\left(L_{\mathrm{dot},3}\right) \rho^{(n)}_{\mathrm{dot},3} d^{\dagger}_{1}\, |0,0\rangle \\
& +\langle 0,0|\, A^{(-)}_{\mathrm{R}}\left(L_{\mathrm{dot},3}\right) \rho^{(n-1)}_{\mathrm{dot},3} d^{\dagger}_{1}\, |0,0\rangle \\
& -\langle 0,0|\, d_{1} \left[A^{(+)}_{\mathrm{L}}\left(L_{\mathrm{dot},3}\right)\right]^{\dagger} \rho^{(n)}_{\mathrm{dot},3}\, |0,0\rangle \\
& -\langle 0,0|\, d_{1} \left[A^{(+)}_{\mathrm{R}}\left(L_{\mathrm{dot},3}\right)\right]^{\dagger} \rho^{(n)}_{\mathrm{dot},3}\, |0,0\rangle \\
& +\langle 0,0|\, d_{1} \rho^{(n)}_{\mathrm{dot},3} \left[A^{(-)}_{\mathrm{L}}\left(L_{\mathrm{dot},3}\right)\right]^{\dagger} |0,0\rangle \\
& +\langle 0,0|\, d_{1} \rho^{(n-1)}_{\mathrm{dot},3} \left[A^{(-)}_{\mathrm{R}}\left(L_{\mathrm{dot},3}\right)\right]^{\dagger} |0,0\rangle\,,
\end{aligned} \tag{5.104}$$

由于

$$d^{\dagger}_{1}\, |0,0\rangle = |1,0\rangle = a_{+}\, |1\rangle^{+} + a_{-}\, |1\rangle^{-}\,, \tag{5.105}$$

$$\langle 0,0|\, d_{1} = \langle 0,1| = a_{+}\, \langle 1|^{+} + a_{-}\, \langle 1|^{-}\,, \tag{5.106}$$

则式 (5.104) 可以进一步表示为

$$\begin{aligned}
\left.\dot{\rho}^{(n)}_{\mathrm{dot},3,00}\right|_{01} = & -a_{+}\, \langle 0,0|\, \rho^{(n)}_{\mathrm{dot},3} A^{(+)}_{\mathrm{L}}\left(L_{\mathrm{dot},3}\right) |1\rangle^{+} \\
& -a_{+}\, \langle 0,0|\, \rho^{(n)}_{\mathrm{dot},3} A^{(+)}_{\mathrm{R}}\left(L_{\mathrm{dot},3}\right) |1\rangle^{+} \\
& -a_{-}\, \langle 0,0|\, \rho^{(n)}_{\mathrm{dot},3} A^{(+)}_{\mathrm{L}}\left(L_{\mathrm{dot},3}\right) |1\rangle^{-} \\
& -a_{-}\, \langle 0,0|\, \rho^{(n)}_{\mathrm{dot},3} A^{(+)}_{\mathrm{R}}\left(L_{\mathrm{dot},3}\right) |1\rangle^{-} \\
& -a_{+}\, \langle 1|^{+} \left[A^{(+)}_{\mathrm{L}}\left(L_{\mathrm{dot},3}\right)\right]^{\dagger} \rho^{(n)}_{\mathrm{dot},3}\, |0,0\rangle \\
& -a_{+}\, \langle 1|^{+} \left[A^{(+)}_{\mathrm{R}}\left(L_{\mathrm{dot},3}\right)\right]^{\dagger} \rho^{(n)}_{\mathrm{dot},3}\, |0,0\rangle \\
& -a_{-}\, \langle 1|^{-} \left[A^{(+)}_{\mathrm{L}}\left(L_{\mathrm{dot},3}\right)\right]^{\dagger} \rho^{(n)}_{\mathrm{dot},3}\, |0,0\rangle
\end{aligned}$$

$$- a_- \langle 1|^- \left[A_{\mathrm{R}}^{(+)}\left(L_{\mathrm{dot},3}\right)\right]^\dagger \rho_{\mathrm{dot},3}^{(n)} |0,0\rangle\,, \tag{5.107}$$

$$\begin{aligned}\dot{\rho}_{\mathrm{dot},3,00}^{(n)}\Big|_{02} =& + a_+ \langle 0,0| A_{\mathrm{L}}^{(-)}\left(L_{\mathrm{dot},3}\right) \rho_{\mathrm{dot},3}^{(n)} |1\rangle^+ \\ & + a_+ \langle 0,0| A_{\mathrm{R}}^{(-)}\left(L_{\mathrm{dot},3}\right) \rho_{\mathrm{dot},3}^{(n-1)} |1\rangle^+ \\ & + a_- \langle 0,0| A_{\mathrm{L}}^{(-)}\left(L_{\mathrm{dot},3}\right) \rho_{\mathrm{dot},3}^{(n)} |1\rangle^- \\ & + a_- \langle 0,0| A_{\mathrm{R}}^{(-)}\left(L_{\mathrm{dot},3}\right) \rho_{\mathrm{dot},3}^{(n-1)} |1\rangle^- \\ & + a_+ \langle 1|^+ \rho_{\mathrm{dot},3}^{(n)} \left[A_{\mathrm{L}}^{(-)}\left(L_{\mathrm{dot},3}\right)\right]^\dagger |0,0\rangle \\ & + a_+ \langle 1|^+ \rho_{\mathrm{dot},3}^{(n-1)} \left[A_{\mathrm{R}}^{(-)}\left(L_{\mathrm{dot},3}\right)\right]^\dagger |0,0\rangle \\ & + a_- \langle 1|^- \rho_{\mathrm{dot},3}^{(n)} \left[A_{\mathrm{L}}^{(-)}\left(L_{\mathrm{dot},3}\right)\right]^\dagger |0,0\rangle \\ & + a_- \langle 1|^- \rho_{\mathrm{dot},3}^{(n-1)} \left[A_{\mathrm{R}}^{(-)}\left(L_{\mathrm{dot},3}\right)\right]^\dagger |0,0\rangle\,,\end{aligned} \tag{5.108}$$

为了计算式 (5.107) 和式 (5.108), 需要对式 (5.96) 求关于时间 $t_1$ 的积分, 其结果可表示为

$$A_\alpha^{(\pm)}\left(L_{\mathrm{dot},3}\right) = \frac{\mathrm{i}\Gamma_\alpha}{2\pi} \int \mathrm{d}\omega \frac{g_\alpha(\omega) f_\alpha^{(\pm)}(\omega)}{\mathrm{i}\eta - \omega - L_{\mathrm{dot},3}} d_1, \tag{5.109}$$

$$\left[A_\alpha^{(\pm)}\left(L_{\mathrm{dot},3}\right)\right]^\dagger = \frac{\mathrm{i}\Gamma_\alpha}{2\pi} \int \mathrm{d}\omega \frac{g_\alpha(\omega) f_\alpha^{(\pm)}(\omega)}{\mathrm{i}\eta + \omega - L_{\mathrm{dot},3}} d_1^\dagger, \tag{5.110}$$

将式 (5.109) 和式 (5.110) 代入式 (5.107) 和式 (5.108), 并利用式 (5.17)～ 式 (5.20), 可得

$$\begin{aligned}\dot{\rho}_{\mathrm{dot},3,00}^{(n)}\Big|_{01} =& -\frac{\mathrm{i}\Gamma_{\mathrm{L}}}{2\pi}\left\{a_+ a_+ \left[I_{1,\mathrm{L}+}(\varepsilon_+) + I_{2,\mathrm{L}+}(\varepsilon_+)\right]\right. \\ & \left. + a_- a_- \left[I_{1,\mathrm{L}+}(\varepsilon_-) + I_{2,\mathrm{L}+}(\varepsilon_-)\right]\right\} \rho_{\mathrm{dot},3,00}^{(n)} \\ & -\frac{\mathrm{i}\Gamma_{\mathrm{R}}}{2\pi}\left\{a_+ a_+ \left[I_{1,\mathrm{R}+}(\varepsilon_+) + I_{2,\mathrm{R}+}(\varepsilon_+)\right]\right. \\ & \left. + a_- a_- \left[I_{1,\mathrm{R}+}(\varepsilon_-) + I_{2,\mathrm{R}+}(\varepsilon_-)\right]\right\} \rho_{\mathrm{dot},3,00}^{(n)},\end{aligned} \tag{5.111}$$

$$\begin{aligned}\dot{\rho}_{\mathrm{dot},3,00}^{(n)}\Big|_{02\text{-}01} =& \; a_+ a_+ \frac{\mathrm{i}\Gamma_{\mathrm{L}}}{2\pi}\left[I_{2,\mathrm{L}-}(\varepsilon_+) + I_{1,\mathrm{L}-}(\varepsilon_+)\right] \rho_{\mathrm{dot},3,++}^{(n)} \\ & + a_+ a_+ \frac{\mathrm{i}\Gamma_{\mathrm{R}}}{2\pi}\left[I_{1,\mathrm{R}-}(\varepsilon_+) + I_{2,\mathrm{R}-}(\varepsilon_+)\right] \rho_{\mathrm{dot},3,++}^{(n-1)},\end{aligned} \tag{5.112}$$

$$\begin{aligned}\dot{\rho}^{(n)}_{\mathrm{dot},3,00}\Big|_{02\text{-}02} &= a_{+}a_{-}\frac{\mathrm{i}\Gamma_{\mathrm{L}}}{2\pi}\left[I_{1,\mathrm{L}-}\left(\varepsilon_{-}\right)+I_{2,\mathrm{L}-}\left(\varepsilon_{+}\right)\right]\rho^{(n)}_{\mathrm{dot},3,+-}\\ &\quad + a_{+}a_{-}\frac{\mathrm{i}\Gamma_{\mathrm{R}}}{2\pi}\left[I_{1,\mathrm{R}-}\left(\varepsilon_{-}\right)+I_{2,\mathrm{R}-}\left(\varepsilon_{+}\right)\right]\rho^{(n-1)}_{\mathrm{dot},3,+-},\end{aligned} \tag{5.113}$$

$$\begin{aligned}\dot{\rho}^{(n)}_{\mathrm{dot},3,00}\Big|_{02\text{-}03} &= a_{+}a_{-}\frac{\mathrm{i}\Gamma_{\mathrm{L}}}{2\pi}\left[I_{1,\mathrm{L}-}\left(\varepsilon_{+}\right)+I_{2,\mathrm{L}-}\left(\varepsilon_{-}\right)\right]\rho^{(n)}_{\mathrm{dot},3,-+}\\ &\quad + a_{+}a_{-}\frac{\mathrm{i}\Gamma_{\mathrm{R}}}{2\pi}\left[I_{1,\mathrm{R}-}\left(\varepsilon_{+}\right)+I_{2,\mathrm{R}-}\left(\varepsilon_{-}\right)\right]\rho^{(n-1)}_{\mathrm{dot},3,-+},\end{aligned} \tag{5.114}$$

$$\begin{aligned}\dot{\rho}^{(n)}_{\mathrm{dot},3,00}\Big|_{02\text{-}04} &= a_{-}a_{-}\frac{\mathrm{i}\Gamma_{\mathrm{L}}}{2\pi}\left[I_{1,\mathrm{L}-}\left(\varepsilon_{-}\right)+I_{2,\mathrm{L}-}\left(\varepsilon_{-}\right)\right]\rho^{(n)}_{\mathrm{dot},3,--}\\ &\quad + a_{-}a_{-}\frac{\mathrm{i}\Gamma_{\mathrm{R}}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{-}\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{-}\right)\right]\rho^{(n-1)}_{\mathrm{dot},3,--}.\end{aligned} \tag{5.115}$$

同理, 可得约化密度矩阵的矩阵元运动方程 $\dot{\rho}^{(n)}_{\mathrm{dot},3,++}$、$\dot{\rho}^{(n)}_{\mathrm{dot},3,+-}$、$\dot{\rho}^{(n)}_{\mathrm{dot},3,-+}$、$\dot{\rho}^{(n)}_{\mathrm{dot},3,--}$ 以及 $\dot{\rho}^{(n)}_{\mathrm{dot},3,11,11}$, 其结果见附录 H.

### 5.4.3 T 型耦合双量子点的电子计数统计性质

在 T 型双量子点中, 两个量子点之间的隧穿耦合强度 $J$ 可以强烈影响 T 型双量子点内电子动力学特性的参数区域, 同样为 $J < (\Gamma_{\mathrm{L}}+\Gamma_{\mathrm{R}})$ 的情形, 因而, 在下面的数值计算中, T 型双量子点的系统参数选为: $\varepsilon_1=\varepsilon_2=1$, $J=0.001$, $U=5$ 和 $k_{\mathrm{B}}T=0.1$, 能量单位为 meV.

对于具有强量子相干性的 T 型双量子点, 在 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}\geqslant 1$ 的情形下, 非马尔可夫效应对电子计数统计特性的影响比串联耦合双量子点更加显著,但是, 在 T 型双量子点中没有观察到负微分电导, 见图 5.8 和图 5.9. 例如, 当 $\Gamma_{\mathrm{L}}/J>1$ 和 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}=1$ 时, 非马尔可夫效应可以进一步增加超泊松散粒噪声的数值, 见图 5.8(b), 并且偏斜度和峭度从一个相对小的正值到一个大负值 (负值的绝对值) 之间的转变可以发生, 尤其是当 $\Gamma_{\mathrm{L}}/J$ 为一个相对大的数值时, 峭度可以进一步被减小到一个非常大的负值, 见图 5.8(c) 和 (d). 对于 $\Gamma_{\mathrm{L}}/J>1$ 和 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}=10$ 的情形, 非马尔可夫效应可以将电流的散粒噪声由次泊松分布转变为超泊松分布, 见图 5.9(b), 并且仅峭度从一个相对小的正值到一个大负值之间的转变可以发生, 见图 5.9(d). 另外, 这里需要指出的是, 与串联耦合双量子点情形相反, 在 T 型双量子点中, 非马尔可夫效应在 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}=1$ 情形下对其电子计数统计特性的影响比 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}>1$ 情形更加明显. 此特性的物理机制起源于 T 型双量子点的电子直接隧穿路径 (隧穿到量子点 1 的传导电子直接隧穿出量子点 1 到达漏极) 和间接隧穿路径 (隧穿到量子点 1 的传导电子先隧穿到量子点 2, 然后再隧穿回量子点 1, 最后再隧穿出量子点 1 到达

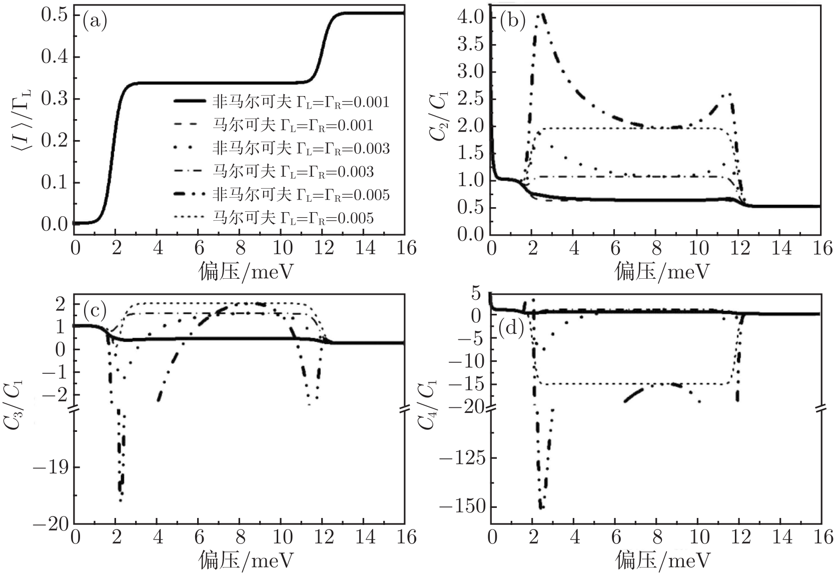


图 5.8 对于 $\Gamma_R$ 为不同数值且 $\Gamma_L/\Gamma_R = 1$ 的情形, T 型双量子点的电流前四阶累积矩, 即 (a) 平均电流 ($\langle I \rangle$)、(b) 散粒噪声 ($C_2/C_1$)、(c) 偏斜度 ($C_3/C_1$)、(d) 峭度 ($C_4/C_1$) 随偏压的变化, 其中 $C_i$ 为电流的第 $i$ 阶零频累积矩

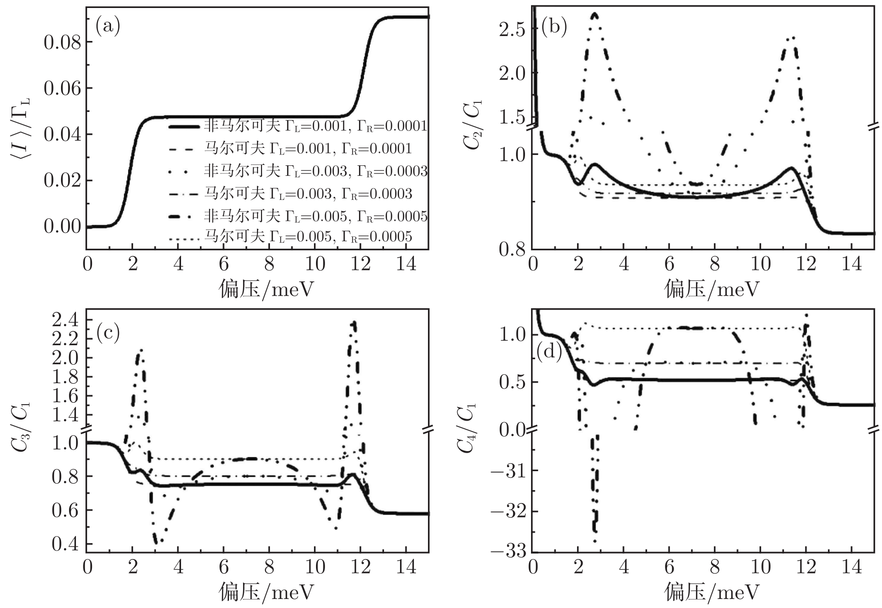


图 5.9 对于 $\Gamma_R$ 为不同数值且 $\Gamma_L/\Gamma_R = 10$ 的情形, T 型双量子点的电流前四阶累积矩, 即 (a) 平均电流 ($\langle I \rangle$)、(b) 散粒噪声 ($C_2/C_1$)、(c) 偏斜度 ($C_3/C_1$)、(d) 峭度 ($C_4/C_1$) 随偏压的变化, 其中 $C_i$ 为电流的第 $i$ 阶零频累积矩

漏极) 之间的量子相干性. 因而, 电子的直接隧穿路径在 $\Gamma_{\mathrm{L}}=10\Gamma_{\mathrm{R}}$ 情形下更容易被压制, 此性质导致非马尔可夫效应在 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}=1$ 情形下对其电子计数统计特性有一个相对大的影响. 对于 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}<1$ 的情形, 与串联耦合双量子点情形相同, 非马尔可夫效应对其电子计数统计特性的影响非常小, 见图 5.10.

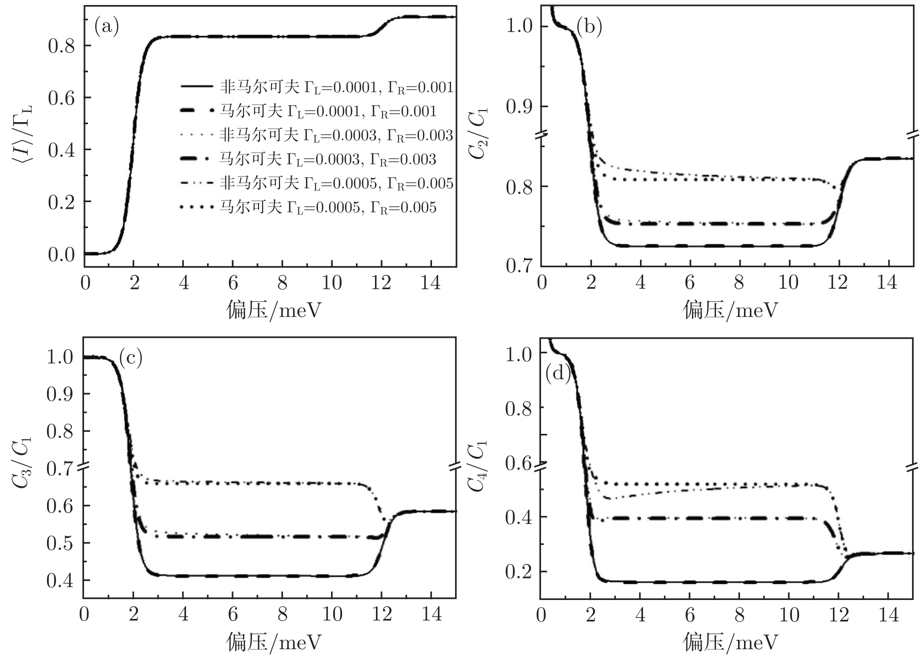


图 5.10 对于 $\Gamma_{\mathrm{R}}$ 为不同数值且 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}=0.1$ 的情形, T 型双量子点的电流前四阶累积矩, 即 (a) 平均电流 ($\langle I\rangle$)、(b) 散粒噪声 ($C_2/C_1$)、(c) 偏斜度 ($C_3/C_1$)、(d) 峭度 ($C_4/C_1$) 随偏压的变化, 其中 $C_i$ 为电流的第 $i$ 阶零频累积矩

为讨论 T 型双量子点电流噪声的物理机制, 在 $\varepsilon_1=\varepsilon_2=\varepsilon\gg J$ 极限下, $\varepsilon_\pm$、$a_\pm$ 和 $b_\pm$ 可以表示为

$$\varepsilon_+=\varepsilon_-=\varepsilon, \tag{5.116}$$

$$a_\pm=\mp\frac{\sqrt{2}}{2},\quad b_\pm=\frac{\sqrt{2}}{2}, \tag{5.117}$$

此时, 约化密度矩阵六个矩阵元的运动方程可以表示为

$$\begin{aligned}\dot{\rho}^{(n)}_{\mathrm{dot},3,00}=&-\left[\Gamma_{\mathrm{L}}f^{(+)}_{\mathrm{L}}(\varepsilon)+\Gamma_{\mathrm{R}}f^{(+)}_{\mathrm{R}}(\varepsilon)\right]\rho^{(n)}_{\mathrm{dot},3,00}\\&+\frac{\Gamma_{\mathrm{L}}}{2}f^{(-)}_{\mathrm{L}}(\varepsilon)\rho^{(n)}_{\mathrm{dot},3,++}+\frac{\Gamma_{\mathrm{R}}}{2}f^{(-)}_{\mathrm{R}}(\varepsilon)\rho^{(n-1)}_{\mathrm{dot},3,++}\\&-\frac{\Gamma_{\mathrm{L}}}{2}f^{(-)}_{\mathrm{L}}(\varepsilon)\rho^{(n)}_{\mathrm{dot},3,+-}-\frac{\Gamma_{\mathrm{R}}}{2}f^{(-)}_{\mathrm{R}}(\varepsilon)\rho^{(n-1)}_{\mathrm{dot},3,+-}\end{aligned}$$

$$
-\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(-)}(\varepsilon)\rho_{\mathrm{dot},3,-+}^{(n)}-\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(-)}(\varepsilon)\rho_{\mathrm{dot},3,-+}^{(n-1)}
+\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(-)}(\varepsilon)\rho_{\mathrm{dot},3,--}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(-)}(\varepsilon)\rho_{\mathrm{dot},3,--}^{(n-1)}, \tag{5.118}
$$

$$
\begin{aligned}
&\dot{\rho}_{\mathrm{dot},3,++}^{(n)}\\
=&\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(+)}(\varepsilon)\rho_{\mathrm{dot},3,00}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(+)}(\varepsilon)\rho_{\mathrm{dot},3,00}^{(n+1)}\\
&-\frac{1}{2}\left\{\Gamma_{\mathrm{L}}\left[f_{\mathrm{L}}^{(+)}(\varepsilon+U)+f_{\mathrm{L}}^{(-)}(\varepsilon)\right]+\Gamma_{\mathrm{R}}\left[f_{\mathrm{R}}^{(+)}(\varepsilon+U)+f_{\mathrm{R}}^{(-)}(\varepsilon)\right]\right\}\rho_{\mathrm{dot},3,++}^{(n)}\\
&+\frac{1}{4\pi}\left[\Gamma_{\mathrm{L}}\left(\mathrm{i}\phi_{\mathrm{L}}-\pi f_{\mathrm{L}}\right)+\Gamma_{\mathrm{R}}\left(\mathrm{i}\phi_{\mathrm{R}}-\pi f_{R}\right)\right]\rho_{\mathrm{dot},3,+-}^{(n)}\\
&-\frac{1}{4\pi}\left[\Gamma_{\mathrm{L}}\left(\mathrm{i}\phi_{\mathrm{L}}+\pi f_{\mathrm{L}}\right)\rho_{\mathrm{dot},3,-+}^{(n)}+\Gamma_{\mathrm{R}}\left(\mathrm{i}\phi_{\mathrm{R}}+\pi f_{\mathrm{R}}\right)\right]\rho_{\mathrm{dot},3,-+}^{(n)}\\
&+\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(-)}(\varepsilon+U)\rho_{\mathrm{dot},3,11,11}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(-)}(\varepsilon+U)\rho_{\mathrm{dot},3,11,11}^{(n-1)},
\end{aligned}\tag{5.119}
$$

$$
\begin{aligned}
&\dot{\rho}_{\mathrm{dot},3,+-}^{(n)}\\
=&-\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(+)}(\varepsilon)\rho_{\mathrm{dot},3,00}^{(n)}-\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(+)}(\varepsilon)\rho_{\mathrm{dot},3,00}^{(n+1)}\\
&+\frac{1}{4\pi}\left[\Gamma_{\mathrm{L}}\left(\mathrm{i}\phi_{\mathrm{L}}-\pi f_{\mathrm{L}}\right)+\Gamma_{\mathrm{R}}\left(\mathrm{i}\phi_{\mathrm{R}}-\pi f_{\mathrm{R}}\right)\right]\rho_{\mathrm{dot},3,++}^{(n)}\\
&-2\mathrm{i}J\rho_{\mathrm{dot},3,+-}^{(n)}\\
&-\frac{1}{2}\left\{\Gamma_{\mathrm{L}}\left[f_{L}^{(+)}(\varepsilon+U)+f_{\mathrm{L}}^{(-)}(\varepsilon)\right]+\Gamma_{\mathrm{R}}\left[f_{\mathrm{R}}^{(+)}(\varepsilon+U)+f_{\mathrm{R}}^{(-)}(\varepsilon)\right]\right\}\rho_{\mathrm{dot},3,+-}^{(n)}\\
&-\frac{1}{4\pi}\left[\Gamma_{\mathrm{L}}\left(\mathrm{i}\phi_{\mathrm{L}}+\pi f_{\mathrm{L}}\right)+\Gamma_{\mathrm{R}}\left(\mathrm{i}\phi_{\mathrm{R}}+\pi f_{\mathrm{R}}\right)\right]\rho_{\mathrm{dot},3,--}^{(n)}\\
&+\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(-)}(\varepsilon+U)\rho_{\mathrm{dot},3,11,11}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(-)}(\varepsilon+U)\rho_{\mathrm{dot},3,11,11}^{(n-1)},
\end{aligned}\tag{5.120}
$$

$$
\begin{aligned}
&\dot{\rho}_{\mathrm{dot},3,-+}^{(n)}\\
=&-\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(+)}(\varepsilon)\rho_{\mathrm{dot},3,00}^{(n)}-\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(+)}(\varepsilon)\rho_{\mathrm{dot},3,00}^{(n+1)}\\
&-\frac{1}{4\pi}\left[\Gamma_{\mathrm{L}}\left(\phi_{\mathrm{L}}+\mathrm{i}\pi f_{\mathrm{L}}\right)+\Gamma_{\mathrm{R}}\left(\phi_{\mathrm{R}}+\mathrm{i}\pi f_{\mathrm{R}}\right)\right]\rho_{\mathrm{dot},3,++}^{(n)}\\
&+2\mathrm{i}J\rho_{\mathrm{dot},3,-+}^{(n)}
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{1}{2}\left\{\Gamma_{\mathrm{L}}\left[f_{\mathrm{L}}^{(+)}(\varepsilon+U)+f_{\mathrm{L}}^{(-)}(\varepsilon)\right]+\Gamma_{\mathrm{R}}\left[f_{\mathrm{R}}^{(+)}(\varepsilon+U)+f_{\mathrm{R}}^{(-)}(\varepsilon)\right]\right\}\rho_{\mathrm{dot},3,-+}^{(n)}\\
&+\frac{1}{4\pi}\left[\Gamma_{\mathrm{L}}\left(\mathrm{i}\phi_{\mathrm{L}}-\pi f_{\mathrm{L}}\right)+\Gamma_{\mathrm{R}}\left(\mathrm{i}\phi_{\mathrm{R}}-\pi f_{\mathrm{R}}\right)\right]\rho_{\mathrm{dot},3,--}^{(n)}\\
&+\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(-)}(\varepsilon+U)\rho_{\mathrm{dot},3,11,11}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(-)}(\varepsilon+U)\rho_{\mathrm{dot},3,11,11}^{(n-1)},
\end{aligned}
\tag{5.121}
$$

$$
\begin{aligned}
\dot{\rho}_{\mathrm{dot},3,--}^{(n)}=&\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(+)}(\varepsilon)\rho_{\mathrm{dot},3,00}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(+)}(\varepsilon)\rho_{\mathrm{dot},3,00}^{(n+1)}\\
&-\frac{1}{4\pi}\left[\Gamma_{\mathrm{L}}\left(\mathrm{i}\phi_{\mathrm{L}}+\pi f_{\mathrm{L}}\right)+\Gamma_{\mathrm{R}}\left(\mathrm{i}\phi_{\mathrm{R}}+\pi f_{\mathrm{R}}\right)\right]\rho_{\mathrm{dot},3,+-}^{(n)}\\
&+\frac{1}{4\pi}\left[\Gamma_{\mathrm{L}}\left(\mathrm{i}\phi_{\mathrm{L}}-\pi f_{\mathrm{L}}\right)+\Gamma_{\mathrm{R}}\left(\mathrm{i}\phi_{\mathrm{R}}-\pi f_{\mathrm{R}}\right)\right]\rho_{\mathrm{dot},3,-+}^{(n)}\\
&-\frac{1}{2}\left\{\Gamma_{\mathrm{L}}\left[f_{\mathrm{L}}^{(+)}(\varepsilon+U)+f_{\mathrm{L}}^{(-)}(\varepsilon)\right]\right.\\
&\left.+\Gamma_{\mathrm{R}}\left[f_{\mathrm{R}}^{(+)}(\varepsilon+U)+f_{\mathrm{R}}^{(-)}(\varepsilon)\right]\right\}\rho_{\mathrm{dot},3,--}^{(n)}\\
&+\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(-)}(\varepsilon+U)\rho_{\mathrm{dot},3,11,11}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(-)}(\varepsilon+U)\rho_{\mathrm{dot},3,11,11}^{(n-1)},
\end{aligned}
\tag{5.122}
$$

$$
\begin{aligned}
\dot{\rho}_{\mathrm{dot},3,11,11}^{(n)}=&\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(+)}(\varepsilon+U)\rho_{\mathrm{dot},3,++}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(+)}(\varepsilon+U)\rho_{\mathrm{dot},3,++}^{(n+1)}\\
&+\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(+)}(\varepsilon+U)\rho_{\mathrm{dot},3,+-}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(+)}(\varepsilon+U)\rho_{\mathrm{dot},3,+-}^{(n+1)}\\
&+\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(+)}(\varepsilon+U)\rho_{\mathrm{dot},3,-+}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(+)}(\varepsilon+U)\rho_{\mathrm{dot},3,-+}^{(n+1)}\\
&+\frac{\Gamma_{\mathrm{L}}}{2}f_{\mathrm{L}}^{(+)}(\varepsilon+U)\rho_{\mathrm{dot},3,--}^{(n)}+\frac{\Gamma_{\mathrm{R}}}{2}f_{\mathrm{R}}^{(+)}(\varepsilon+U)\rho_{\mathrm{dot},3,--}^{(n+1)}\\
&-\Gamma_{\mathrm{L}}f_{\mathrm{L}}^{(-)}(\varepsilon+U)\rho_{\mathrm{dot},3,11,11}^{(n)}-\Gamma_{\mathrm{R}}f_{\mathrm{R}}^{(-)}(\varepsilon+U)\rho_{\mathrm{dot},3,11,11}^{(n)}.
\end{aligned}
\tag{5.123}
$$

由式 (5.118)~式 (5.123) 可知, T 型双量子点的上述电流噪声特性同样起源于其量子相干性, 并且可以用函数 $\phi_{\mathrm{L}}+0.1\phi_{\mathrm{R}}$ 和 $\phi_{\mathrm{L}}+\phi_{\mathrm{R}}$ 随偏压的数值变化理解. 例如, 对于选取的 T 型双量子点参数, 由图 5.6(b) 可知, 函数 $\phi_{\mathrm{L}}+0.1\phi_{\mathrm{R}}$ 和 $\phi_{\mathrm{L}}+\phi_{\mathrm{R}}$ 的数值在有新的电子输运通道开始参与量子输运的偏压 $V_{\mathrm{b}}=2$ 和 $V_{\mathrm{b}}=12$ 附近呈现出一个非常明显的变化; 但是, 对于 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}<1$ 的情形, 函数 $0.1\phi_{\mathrm{L}}+\phi_{\mathrm{R}}$ 的数值随着偏压的增大呈现出一个比较缓慢的变化.

## 5.5 结　论

基于时间局域的粒子数分辨量子主方程, 在顺序隧穿极限下, 通过三个典型的量子点体系, 即无量子相干性的单量子点、量子相干性可调的串联耦合双量子点和 T 型双量子点, 发现非马尔可夫效应通过开放量子系统的量子相干性体现. 特别是, 对于具有强量子相干性的开放量子系统, 非马尔可夫效应对其电子全计数统计有明显的影响, 但这种影响依赖于单分子体系与源极和漏极的耦合强度. 因此, 对于具有强量子相干性的开放量子系统, 非马尔可夫效应对其电子全计数统计的影响将不能忽略. 此特性可以为理解开放量子系统的电子输运特性的物理机制提供进一步的信息.

## 参 考 文 献

[1] Levitov L S, Lee H, Lesovik G B. Electron counting statistics and coherent states of electric current. J. Math. Phys., 1996, 37: 4845-4866.

[2] Blanter Y M, Büttiker M. Shot noise in mesoscopic conductors. Phys. Rep., 2000, 336: 1-166.

[3] Nazarov Y V. Quantum Noise in Mesoscopic Physics. Dordrecht: Springer, 2003.

[4] Gustavsson S, Leturcq R, Simovič B, et al. Counting statistics of single electron transport in a quantum dot. Phys. Rev. Lett., 2006, 96: 076605.

[5] Fujisawa T, Hayashi T, Tomita R, et al. Bidirectional counting of single electrons. Science, 2006, 312: 1634-1636.

[6] Flindt C, Fricke C, Hohls F, et al. Universal oscillations in counting statistics. Proc. Natl. Acad. Sci. U.S.A., 2009, 106: 10116-10119.

[7] Fricke C, Hohls F, Sethubalasubramanian N, et al. High-order cumulants in the counting statistics of asymmetric quantum dots. Appl. Phys. Lett., 2010, 96: 202103.

[8] Ubbelohde N, Fricke C, Flindt C, et al. Measurement of finite-frequency current statistics in a single-electron transistor. Nat. Comms., 2012, 3: 612.

[9] Fricke L, Wulf M, Kaestner B, et al. Counting statistics for electron capture in a dynamic quantum dot. Phys. Rev. Lett., 2013, 110: 126803.

[10] Maisi V F, Kambly D, Flindt C, et al. Full counting statistics of Andreev tunneling. Phys. Rev. Lett., 2014, 112: 036801.

[11] Aguado R, Brandes T. Shot noise spectrum of open dissipative quantum two-level systems. Phys. Rev. Lett., 2004, 92: 206601.

[12] Kießlich G, Schöll E, Brandes T, et al. Noise enhancement due to quantum coherence in coupled quantum dots. Phys. Rev. Lett., 2007, 99: 206602.

[13] Yamauchi Y, Sekiguchi K, Chida K, et al. Evolution of the kondo effect in a quantum dot probed by shot noise. Phys. Rev. Lett., 2011, 106: 176601.

[14] Vardimon R, Klionsky M, Tal O. Experimental determination of conduction channels in atomic-scale conductors based on shot noise measurements. Phys. Rev. B, 2013, 88: 161404(R).

[15] Kubo T, Tokura Y, Tarucha S. Kondo effects and shot noise enhancement in a laterally coupled double quantum dot. Phys. Rev. B, 2011, 83: 115310.

[16] Meair J, Stano P, Jacquod P. Measuring spin accumulations with current noise. Phys. Rev. B, 2011, 84: 073302.

[17] Milletarì M, Rosenow B. Shot-noise signatures of charge fractionalization in the $\nu$=2 quantum hall edge. Phys. Rev. Lett., 2013, 111: 136807.

[18] Bodoky F, Belzig W, Bruder C. Connection between noise and quantum correlations in a double quantum dot. Phys. Rev. B, 2008, 77: 035302.

[19] Dubrovin D, Eisenberg E. Super-Poissonian shot noise as a measure of dephasing in closed quantum dots. Phys. Rev. B, 2007, 76: 195330.

[20] Xue H B, Nie Y H, Li Z J, et al. Tunable electron counting statistics in a single-molecule magnet. J. Appl. Phys., 2010, 108: 033707.

[21] Xue H B, Nie Y H, Li Z J, et al. Effect of finite Coulomb interaction on full counting statistics of electronic transport through single-molecule magnet. Phys. Lett. A, 2011, 375: 716-725.

[22] Blum K. Density Matrix Theory and Applications. 3rd ed. Dordrecht : Springer, 2012.

[23] Gurvitz S A, Prager Y S. Microscopic derivation of rate equations for quantum transport. Phys. Rev. B, 1996, 53: 15932-15943.

[24] Braun M, König J, Martinek J. Theory of transport through quantum-dot spin valves in the weak-coupling regime. Phys. Rev. B, 2004, 70: 195345.

[25] Wunsch B, Braun M, König J, et al. Probing level renormalization by sequential transport through double quantum dots. Phys. Rev. B, 2005, 72: 205319.

[26] Djuric I, Dong B, Cui H L. Super-Poissonian shot noise in the resonant tunneling due to coupling with a localized level. Appl. Phys. Lett., 2005, 87: 032105.

[27] Djuric I, Dong B, Cui H L. Theoretical investigations for shot noise in correlated resonant tunneling through a quantum coupled system. J. Appl. Phys., 2006, 99: 063710.

[28] Harbola U, Esposito M, Mukamel S. Quantum master equation for electron transport through quantum dots and single molecules. Phys. Rev. B, 2006, 74: 235309.

[29] Pedersen J N, Lassen B, Wacker A, et al. Coherent transport through an interacting double quantum dot: Beyond sequential tunneling. Phys. Rev. B, 2007, 75: 235314.

[30] Begemann G, Darau D, Donarini A, et al. Symmetry fingerprints of a benzene single-electron transistor: Interplay between Coulomb interaction and orbital symmetry. Phys. Rev. B, 2008, 77: 201406(R).

[31] Darau D, Begemann G, Donarini A, et al. Interference effects on the transport characteristics of a benzene single-electron transistor. Phys. Rev. B, 2009, 79: 235404.

[32] Schultz M G, von Oppen F. Quantum transport through nanostructures in the singular-coupling limit. Phys. Rev. B, 2009, 80: 033302.

[33] Schaller G, Kießlich G, Brandes T. Transport statistics of interacting double dot systems: Coherent and non-Markovian effects. Phys. Rev. B, 2009, 80: 245107.

[34] Kießlich G, Samuelsson P, Wacker A, et al. Counting statistics and decoherence in coupled quantum dots. Phys. Rev. B, 2006, 73: 033312.

[35] Xue H B. Full counting statistics as a probe of quantum coherence in a side-coupled double quantum dot system. Ann. Phys. (New York), 2013, 339: 208-217.

[36] Welack S, Esposito M, Harbola U, et al. Interference effects in the counting statistics of electron transfers through a double quantum dot. Phys. Rev. B, 2008, 77: 195315.

[37] Fang T F, Wang S J, Zuo W. Flux-dependent shot noise through an Aharonov-Bohm interferometer with an embedded quantum dot. Phys. Rev. B, 2007, 76: 205312.

[38] Fang T F, Zuo W, Chen J Y. Fano effect on shot noise through a Kondo-correlated quantum dot. Phys. Rev. B, 2008, 77: 125136.

[39] Braggio A, König J, Fazio R. Full counting statistics in strongly interacting systems: Non-Markovian effects. Phys. Rev. Lett., 2006, 96: 026805.

[40] Flindt C, Novotný T, Braggio A, et al. Counting statistics of non-Markovian quantum stochastic processes. Phys. Rev. Lett., 2008, 100: 150601.

[41] Zedler P, Schaller G, Kiesslich G, et al. Weak-coupling approximations in non-Markovian transport. Phys. Rev. B, 2009, 80: 045309.

[42] Emary C. Counting statistics of cotunneling electrons. Phys. Rev. B, 2009, 80: 235306.

[43] Flindt C, Novotný T, Braggio A, et al. Counting statistics of transport through Coulomb blockade nanostructures: High-order cumulants and non-Markovian effects. Phys. Rev. B, 2010, 82: 155407.

[44] Marcos D, Emary C, Brandes T, et al. Non-Markovian effects in the quantum noise of interacting nanostructures. Phys. Rev. B, 2011, 83:125426.

[45] Emary C, Aguado R. Quantum versus classical counting in non-Markovian master equations. Phys. Rev. B, 2011, 84: 085425.

[46] Zedler P, Emary C, Brandes T, et al. Noise calculations within the second-order von Neumann approach. Phys. Rev. B, 2011, 84: 233303.

[47] Li X Q, Luo J, Yang Y G, et al. Quantum master-equation approach to quantum transport through mesoscopic systems. Phys. Rev. B, 2005, 71: 205304.

[48] Wang S K, Jiao H J, Li F, et al. Full counting statistics of transport through two-channel Coulomb blockade systems. Phys. Rev. B, 2007, 76: 125416.

[49] Elzerman J M, Hanson R, Willems van Beveren L H, et al. Single-shot read-out of an individual electron spin in a quantum dot. Nature, 2004, 430: 431-435.

[50] Xue H B, Zhang Z X, Fei H M. Tunable super-Poissonian noise and negative differential conductance in two coherent strongly coupled quantum dots. Eur. Phys. J. B, 2012, 85: 336.

[51] Stoof T H, Nazarov Y V. Time-dependent resonant tunneling via two discrete states. Phys. Rev. B, 1996, 53: 1050-1053.

# 第 6 章　非马尔可夫电子计数统计理论的应用：共隧穿

在单分子的电子输运实验中, 单分子与源极、漏极的隧穿耦合强度通常处于中间耦合强度区域, 此时, 电子的共隧穿过程将成为影响其输运特性的另一个重要因素. 在本章中, 将基于四阶时间局域的粒子数分辨量子主方程, 以 T 型双量子点为例, 给出共隧穿辅助顺序隧穿过程的电子计数统计的计算流程, 并讨论其前四阶电流累积矩的特性, 最后, 给出在共隧穿极限下, 开放量子系统非马尔可夫电子计数统计与其系统量子相干性以及共隧穿过程之间的关系.

## 6.1　引　　言

在一个开放量子系统中, 当量子系统与电子库之间的隧穿耦合强度处于中间耦合强度区域时, 高阶电子隧穿过程, 如共隧穿过程, 将影响开放量子系统的电子输运性质并产生一些新奇的物理特性. 因此, 开放量子系统, 尤其是称之为人造分子的量子点系统和单分子中的电子共隧穿在实验 [1-6] 和理论 [7-12] 上引起极大的关注和研究兴趣. 其中, 量子点系统的共隧穿散粒噪声 [13-28] 和全计数统计 [26,29-31], 因其可以揭示平均电流无法提供的关于量子系统的本质特性和电子关联信息, 引起人们的极大关注. 例如, 在电子传输主要由共隧穿过程决定的库仑阻塞区域内, 实验和理论均已证明输运电流的散粒噪声为超泊松分布.

另外,在强相干的量子系统中,量子相干性在电子隧穿过程中起重要作用[28,32-38]. 特别是, 非马尔可夫效应在电子非平衡隧穿过程中也起着重要作用 [39], 并且通过系统的量子相干性体现 [38]. 因而, 对于量子系统与电子库之间的隧穿耦合强度处于中间耦合强度区域的情形, 一个开放量子系统的电子隧穿过程主要由电子的顺序隧穿、共隧穿以及系统的量子相干性之间的相互竞争或者相互作用决定. 在库仑阻塞区域内, 电子隧穿主要通过共隧穿过程进行; 但是, 在电子隧穿主要通过顺序隧穿过程进行的顺序隧穿区域, 共隧穿过程对系统的微分电导和散粒噪声影响很小 [3,27,39,40]. 在库仑阻塞区域到顺序隧穿区域的过渡区域和顺序隧穿区域, 理论研究已经证明, 电子的共隧穿辅助顺序隧穿过程对开放量子系统的微分电导和散粒噪声有重要影响. 但是, 在顺序隧穿区域内, 电子的共隧穿辅助顺序隧穿过程和系统的量子相干性对其非马尔可夫电子全计数统计的影响依然是一个开放的课题且尚

未被揭示.

在本章中, 将基于共隧穿极限下的时间局域的粒子数分辨量子主方程, 以量子相干性可调的 T 型双量子点 (其哈密顿量已在第 5 章中介绍, 这里不再赘述) 为例, 在顺序隧穿区域内, 研究电子的共隧穿过程和 T 型双量子点的量子相干性对其非马尔可夫电子全计数统计的影响.

## 6.2 T 型双量子点的共隧穿辅助顺序隧穿的偏压区域

对于开放 T 型双量子点系统, 可以通过调节两个量子点之间的隧穿耦合强度 $J$ 相对于量子点 1 与源极、漏极的隧穿耦合强度 $\Gamma=\Gamma_{\rm L}+\Gamma_{\rm R}$ 的数值来改变其量子相干性. 在 $J\ll\Gamma$ 情形下, 两个量子点之间的隧穿耦合强度 $J$ 可以强烈影响 T 型双量子点的电子动力学特性, 此时, 该系统约化密度矩阵的非对角元在电子隧穿过程中起关键作用 [35,38,41]. 但是, 对于 $J\gg\Gamma$ 的情形, 该系统约化密度矩阵的非对角元在电子隧穿过程中影响很小, 此时, 约化密度矩阵的对角元在电子隧穿过程中起关键作用 [35]. 由于在本章中重点讨论量子相干性和电子共隧穿过程对其共隧穿辅助顺序隧穿过程电子计数统计的影响, 因而, 选择量子相干性对其电子隧穿过程影响比较大的偏压区域, 即当两个单电子占据态到空占据态之间的转变仅参与电子输运的偏压区域. 对于本章选择的 T 型双量子点参数 (能量单位为 meV)[42], 即 $\varepsilon_1=\varepsilon_2=2.35$, $U=4$ 和 $k_{\rm B}T=0.1$(除非另外特殊说明), 在下面的数值计算中, 偏压区域选取为 $V_{\rm b}=4.5$. 为了确定共隧穿辅助顺序隧穿过程电子计数统计对量子相干性和电子共隧穿过程的依赖关系, 考虑 T 型双量子点的平均电流、散粒噪声、偏斜度和峭度随着隧穿耦合强度 $\Gamma_\alpha$ 在如下四种情形下的变化: ① 仅考虑顺序隧穿过程约化密度矩阵的对角元, 以 “二阶对角元” 标记; ② 考虑顺序隧穿过程约化密度矩阵的对角元和非对角元, 以 “二阶非对角元” 标记; ③ 仅考虑共隧穿辅助顺序隧穿的对角元, 以 “四阶对角元” 标记; ④ 考虑共隧穿辅助顺序隧穿的对角元和非对角元, 以 “四阶非对角元” 标记. 另外, 为了方便读者验证相关过程的推导, 在本附录 I 中, 给出了描述电子共隧穿过程的矩阵元运动方程 $\dot{\rho}^{(n)}_{\rm S,co,00}(t)$ 的推导.

## 6.3 强量子相干性的 T 型双量子点

对于两个量子点之间的隧穿耦合强度 $J$ 可以强烈影响 T 型双量子点的电子动力学特性的情形, 即 $J\ll\Gamma$, 对于上面选择的 T 型双量子点参数, 两个量子点之间的隧穿耦合强度选取为 $J=0.001$.

### 6.3.1 T 型耦合双量子点的温度效应

为了研究 T 型双量子点的系统温度对其电流前四阶累积矩的影响, 下面从量

子点与源极、漏极的不对称耦合, 即 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}} > 1$ 和 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}} \leqslant 1$ 两种情形讨论. 对于 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}} > 1$ 的情形, 当 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}} = 10$ 时, 图 6.1 给出了 T 型双量子点的电流前四阶累积矩在不同温度情形下随着隧穿耦合强度 $\Gamma_{\mathrm{L}}$ 的变化. 在 $\Gamma/J < 1$ 情形下, 电子的共隧穿过程起主要作用, 并且决定了散粒噪声和高阶累积矩的数值大小; 而当 $\Gamma/J \gg 1$ 时, 系统的量子相干性起主要作用, 并且决定了散粒噪声、偏斜度以及峭度的 Fano 因子是否大于 1, 见图 6.1. 对于 $\Gamma/J$ 为中间数值时, 共隧穿过程和量子相干性的相互竞争发生, 从而导致形成一个过渡区域, 但是此区域的大小依赖于系统的温度, 见图 6.1.

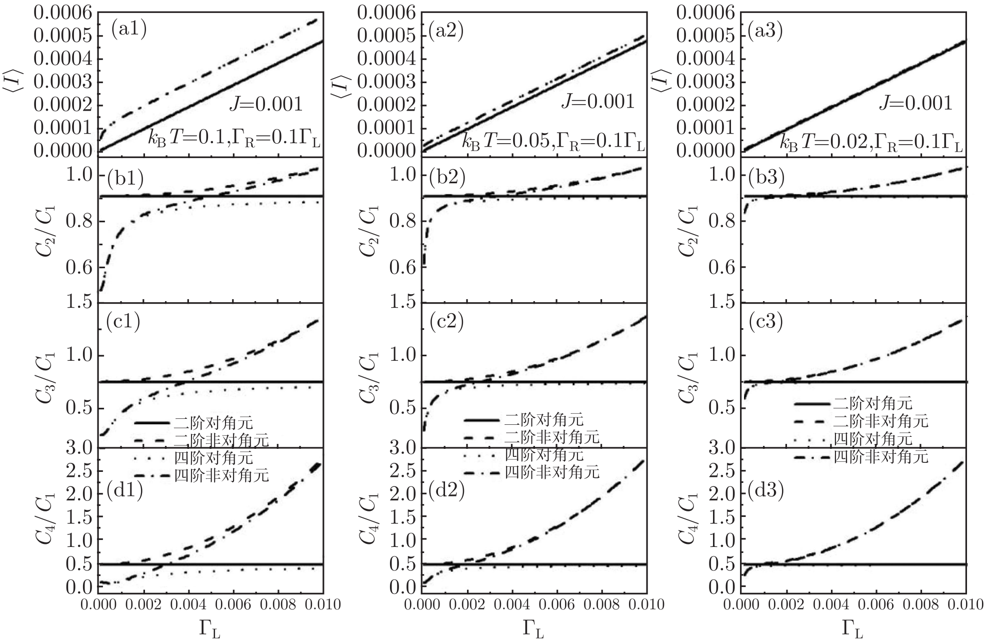


图 6.1 当 $\Gamma_{\mathrm{R}} = 0.1\Gamma_{\mathrm{L}}$ 时, T 型双量子点的电流前四阶累积矩, 即 (a1)~(a3) 平均电流 ($\langle I \rangle$)、(b1)~(b3) 散粒噪声 ($C_2/C_1$)、(c1)~(c3) 偏斜度 ($C_3/C_1$)、(d1)~(d3) 峭度 ($C_4/C_1$) 在不同温度情形下随隧穿耦合强度 $\Gamma_{\mathrm{L}}$ 的变化, 其中 $C_i$ 为电流的第 $i$ 阶零频累积矩. T 型双量子点的其他参数见图中说明

对于 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}} \leqslant 1$ 的情形, 由共隧穿过程和量子相干性之间相互竞争形成的过渡区域的大小非常小, 见图 6.2 和图 6.3. 尤其是, 当 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}} \leqslant 1$ 和 $\Gamma/J \gg 1$ 时, 共隧穿过程和量子相干性的相互作用决定了传输电子数目的计数统计特性, 例如, 散粒噪声的超泊松分布是否发生, 以及偏斜度和峭度的 Fano 因子是否从一个正值转变为一个负值, 见图 6.2 和图 6.3. 由于偏斜度和峭度的数值大小和正负分别刻画了一段时间间隔 $t$ 内电子数在平均传输电子数目 $\bar{n}$ 附近分布的不对称性和其分布

峰的峭度, 因而, 偏斜度和峭度可以提供超越散粒噪声的关于电子计数统计的进一步信息. 此外, 在 $\Gamma_{\rm L}/\Gamma_{\rm R}=1$ 和 $\Gamma/J\gg 1$ 情形下, 电流的散粒噪声特性主要由其系统的量子相干性决定, 见图 6.3. 同样, 这些电流累积矩的特性依赖于其系统温度, 即随着系统温度的降低量子相干性将在电子隧穿过程中起决定性作用.

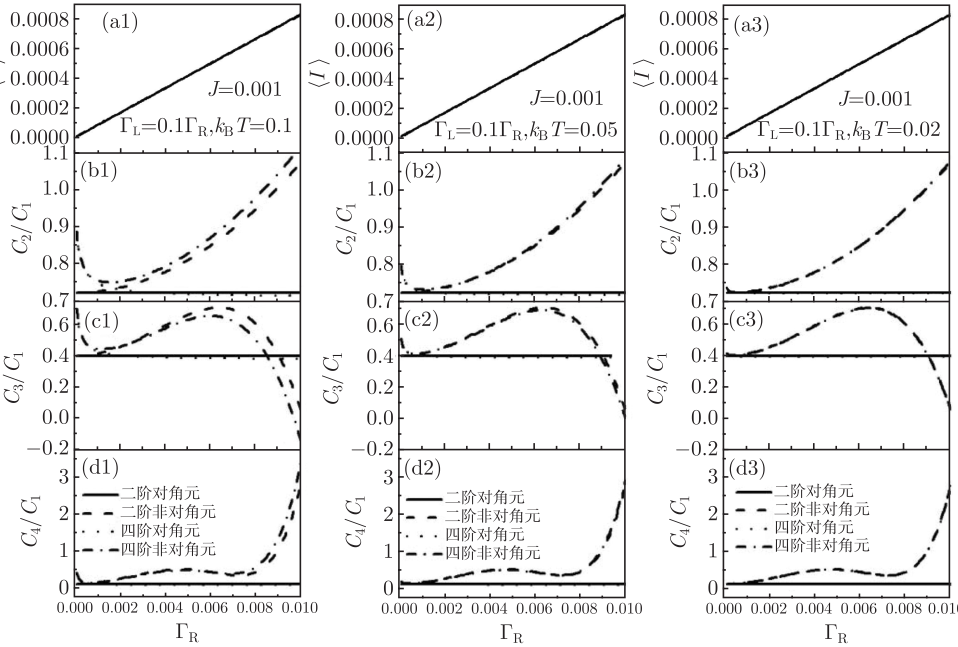


图 6.2 当 $\Gamma_{\rm L}=0.1\Gamma_{\rm R}$ 时, T 型双量子点的电流前四阶累积矩, 即 (a1)~(a3) 平均电流 ($\langle I\rangle$)、(b1)~(b3) 散粒噪声 ($C_2/C_1$)、(c1)~(c3) 偏斜度 ($C_3/C_1$)、(d1)~(d3) 峭度 ($C_4/C_1$) 在不同温度情形下随隧穿耦合强度 $\Gamma_{\rm R}$ 的变化, 其中 $C_i$ 为电流的第 $i$ 阶零频累积矩. T 型双量子点的其他参数见图中说明

上面讨论的温度对 T 型双量子点电流前四阶累积矩的影响可以用共隧穿过程诱导的本征态占据概率的重新分布来理解. 对于 $\Gamma_{\rm L}/\Gamma_{\rm R}=10$ 的情形, 两个单电子本征态的占据概率远大于空占据态, 见图 6.4(a1)~(a3), 因而, 电子在隧穿出量子点 1 到达漏极之前会在 T 型双量子点内有一个比较长的停留时间. 当 $\Gamma/J\ll 1$ 时, 传导电子将在两个单电子本征态之间快速地来回隧穿, 因而, 增加了由双电子占据态 $|1,1\rangle$ 与两个单电子本征态 $|1\rangle^{\pm}$ 之间转变诱导的共隧穿过程发生的概率. 因此, 共隧穿过程可以使两个单电子本征态和空占据态的占据概率随着 $\Gamma/J$ 数值的减小分别大幅减小和增大, 见图 6.4(a1)~(a3). 相应地, 由顺序隧穿诱导的电子隧穿阻塞被上面的共隧穿过程解除, 从而导致电流的散粒噪声被减小, 见图 6.1(b1)~(b3).

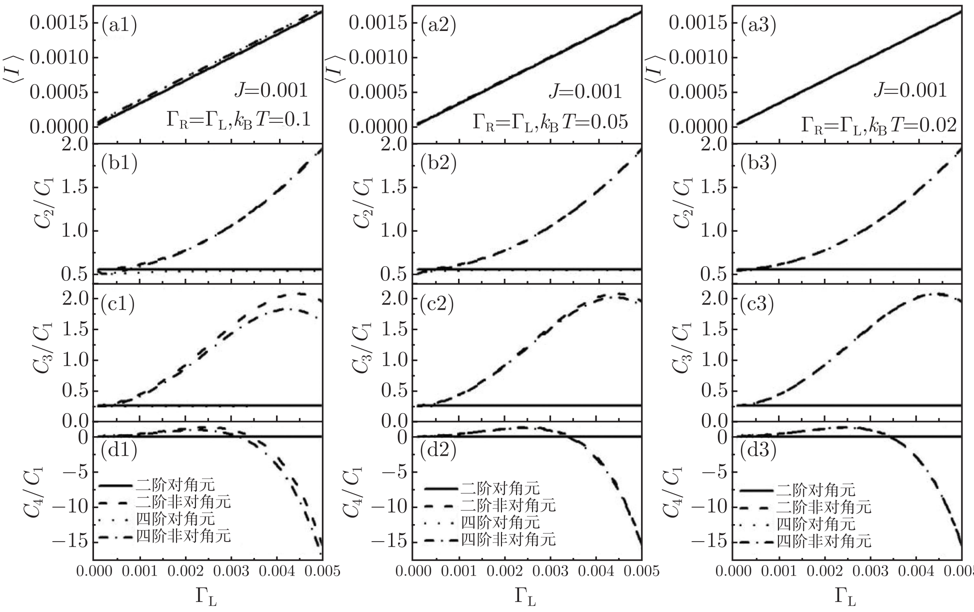


图 6.3　当 $\Gamma_L = \Gamma_R$ 时, T 型双量子点的电流前四阶累积矩, 即 (a1)～(a3) 平均电流 ($\langle I\rangle$)、(b1)～(b3) 散粒噪声 ($C_2/C_1$)、(c1)～(c3) 偏斜度 ($C_3/C_1$)、(d1)～(d3) 峭度 ($C_4/C_1$) 在不同温度情形下随隧穿耦合强度 $\Gamma_L$ 的变化, 其中 $C_i$ 为电流的第 $i$ 阶零频累积矩. T 型双量子点的其他参数见图中说明

但是, 当 $\Gamma/J \gg 1$ 时, 传导电子在两个单电子本征态之间隧穿的速度非常慢, 从而压制了共隧穿过程, 此时, 共隧穿过程对两个单电子本征态和空占据态占据概率的重新分布影响很小, 见图 6.4(a1)～(a3). 因而, 系统的量子相干性在电子隧穿过程中起主要作用. 与上面的 $\Gamma_L/\Gamma_R = 10$ 情形不同, 对于 $\Gamma_L/\Gamma_R = 0.1$ 的情形, 两个单电子本征态的占据概率远小于空占据态, 因而, 电子在 T 型双量子点内的停留时间非常短. 对于 $\Gamma/J \gg 1$ 的情形, 双电子隧穿过程可以通过由双电子占据态 $|1,1\rangle$ 与两个单电子本征态 $|1\rangle^{\pm}$ 之间转变诱导的共隧穿过程以及随后由两个单电子本征态 $|1\rangle^{\pm}$ 与空占据态之间转变诱导的顺序隧穿过程, 这两个连续的电子隧穿过程进行. 此时, 电子的共隧穿辅助顺序隧穿过程在 $\Gamma/J \gg 1$ 情形下对其电子计数统计特性起重要作用, 因而形成一个共隧穿过程和量子相干性共同对其电子计数统计特性起重要作用的区域. 但是, 上面讨论的共隧穿过程诱导的本征态占据概率的非平衡分布依赖于系统的温度, 即系统温度越低, 共隧穿过程对两个单电子本征态和空占据态占据概率重新分布的影响就越小. 因而, 随着温度的降低, 温度对其电子计数统计特性的影响将越来越小. 另外, 共隧穿过程在 $\Gamma/J \ll 1$ 情形下随着 $\Gamma/J$ 数值的减小可以进一步增加空占据态的概率, 见图 6.4(b1)～(b3), 此效应可以进一步增加

电子隧穿过程被阻塞的概率, 相应的电流的散粒噪声被增大, 见图 6.2(b1)～(b3).

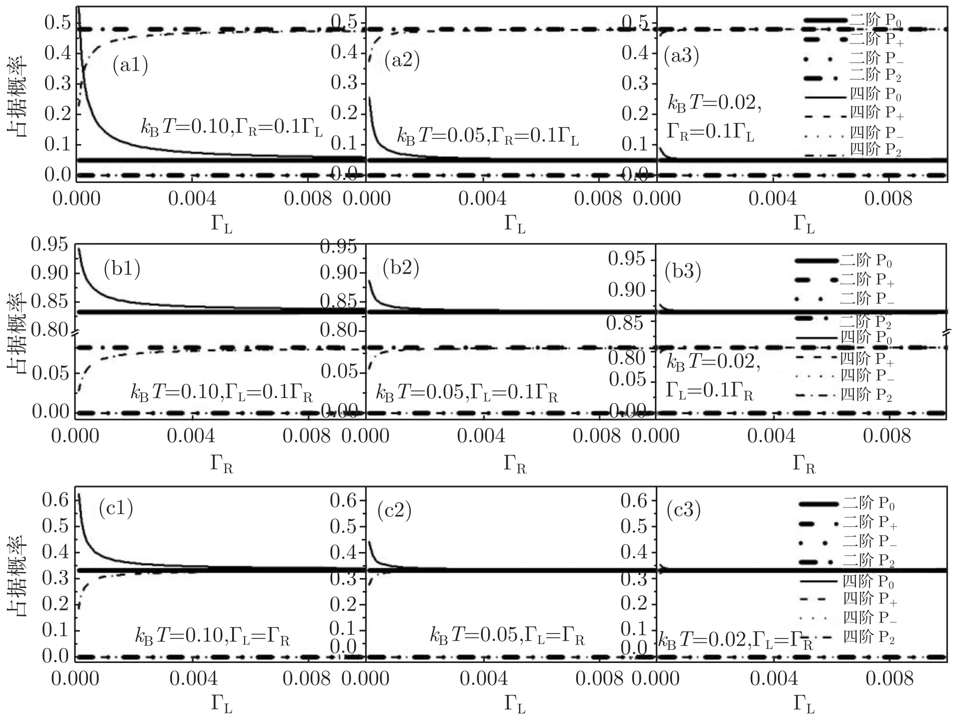


图 6.4　T 型双量子点本征态的占据概率在不同温度和 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}$ 为不同数值情形下随隧穿耦合强度 $\Gamma_{\mathrm{L}}(\Gamma_{\mathrm{R}})$ 的变化, 其中图 (a1)～(a3)、图 (b1)～(b3) 和图 (c1)～(c3) 分别与图 6.1、图 6.2 和图 6.3 的参数相同

### 6.3.2　T 型耦合双量子点与源极、漏极的不对称耦合效应

在本节中, 在给定系统温度情形下, 即 $k_{\mathrm{B}}T = 0.1$, 研究量子点与源极、漏极的不对称耦合 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}$ 对其电流前四阶累积矩的影响. 当 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}} > 1$ 且 $\Gamma/J$ 为中间数值时, 对于 Fano 因子被共隧穿过程减小而被量子相干性增加的过渡区域, 其大小随着 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}$ 数值的增加而变大, 见图 6.5. 但是, 当 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}} < 1$ 且 $\Gamma/J \gg 1$ 时, 共隧穿过程和量子相干性之间的相互作用随着 $\Gamma_{\mathrm{R}}/\Gamma_{\mathrm{L}}$ 数值的减小对其电子计数统计特性有一个更加明显的影响. 例如, 散粒噪声和峭度的 Fano 因子的数值是否大于 1, 以及偏斜度的数值从正值到负值的转变能否发生, 见图 6.6. 这些结果同样可以用量子点与源极、漏极的不对称耦合 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}$ 诱导的本征态占据概率的重新分布来理解, 见图 6.7.

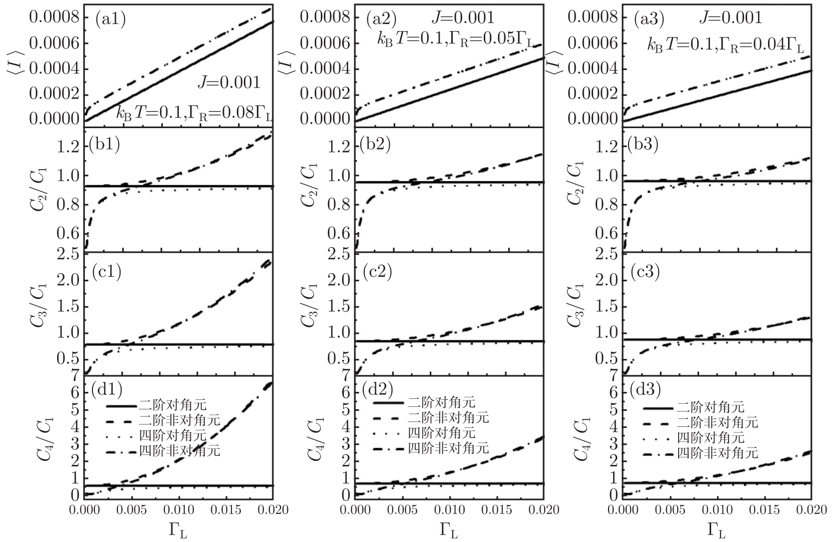


图 6.5 当 $k_{\mathrm{B}}T=0.1$ 时, T 型双量子点的电流前四阶累积矩, 即 (a1)～(a3) 平均电流 ($\langle I\rangle$)、(b1)～(b3) 散粒噪声 ($C_2/C_1$)、(c1)～(c3) 偏斜度 ($C_3/C_1$)、(d1)～(d3) 峭度 ($C_4/C_1$) 在 $\Gamma_{\mathrm{R}}/\Gamma_{\mathrm{L}}$为不同数值情形下随隧穿耦合强度 $\Gamma_{\mathrm{L}}$ 的变化, 其中 $C_i$ 为电流的第 $i$ 阶零频累积矩

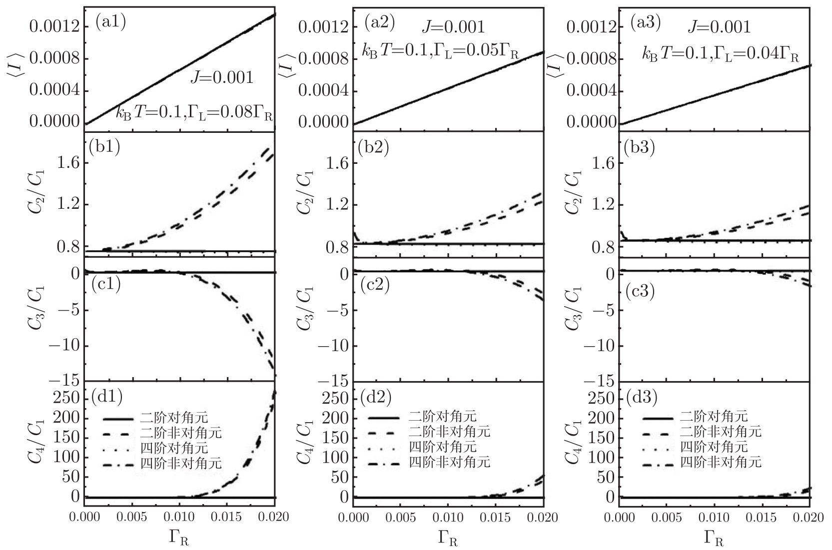


图 6.6 当 $k_{\mathrm{B}}T=0.1$ 时, T 型双量子点的电流前四阶累积矩, 即 (a1)～(a3) 平均电流 ($\langle I\rangle$)、(b1)～(b3) 散粒噪声 ($C_2/C_1$)、(c1)～(c3) 偏斜度 ($C_3/C_1$)、(d1)～(d3) 峭度 ($C_4/C_1$) 在 $\Gamma_{\mathrm{L}}/\Gamma_{\mathrm{R}}$为不同数值情形下随隧穿耦合强度 $\Gamma_{\mathrm{R}}$ 的变化, 其中 $C_i$ 为电流的第 $i$ 阶零频累积矩

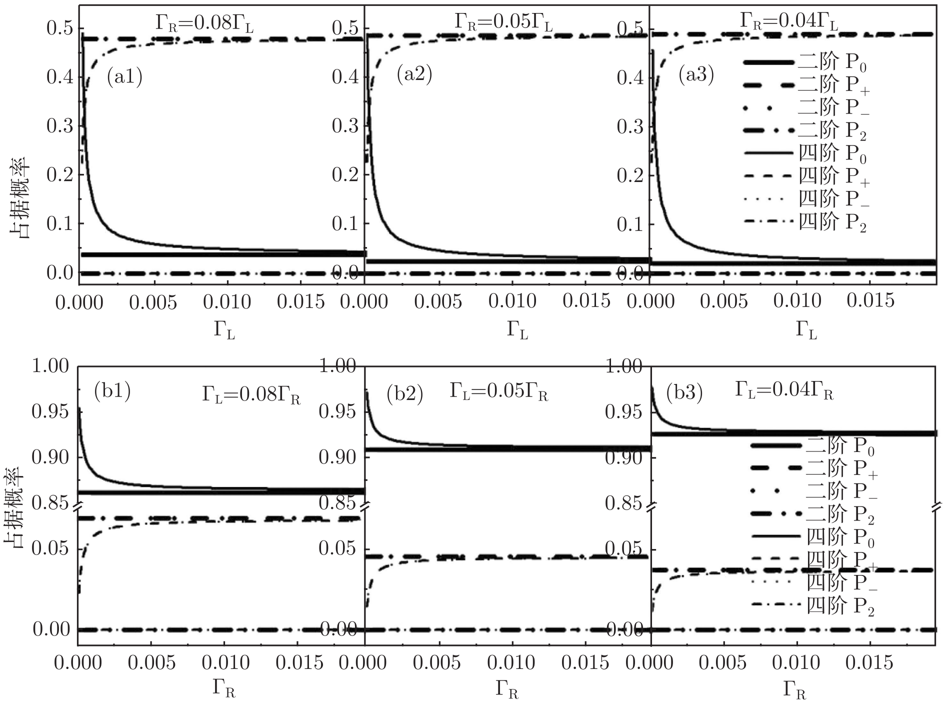


图 6.7 T 型双量子点本征态的占据概率在 $\Gamma_L/\Gamma_R$ 为不同数值情形下随隧穿耦合强度 $\Gamma_L(\Gamma_R)$ 的变化, 其中图 (a1)~(a3) 和 (b1)~(b3) 分别与图 6.5 和图 6.6 的参数相同

## 6.4 弱量子相干性的 T 型双量子点

现在, 讨论共隧穿过程对具有弱量子相干性的开放 T 型双量子点系统中电子计数统计特性的影响. 对于本章选择的 T 型双量子点参数, 此时, 两个量子点之间的隧穿耦合强度选取为 $J=1$, 并且选择如下三个固定的偏压: ① 仅单电子本征态 $|1\rangle^-$ 到空占据态之间的转变参与量子输运的偏压区域, 即 $V_b=2.5$; ② 两个单电子本征态 $|1\rangle^\pm$ 到空占据态之间的转变参与量子输运的偏压区域, 即 $V_b=4.5$; ③ 两个单电子本征态 $|1\rangle^\pm$ 到空占据态之间的转变以及双电子占据态 $|1,1\rangle$ 与单电子本征态 $|1\rangle^+$ 之间的转变参与量子输运的偏压区域, 即 $V_b=6.5$. 由图 6.8 和图 6.9 可知, 传输电子数目的前四阶电流累积矩可以由共隧穿过程很好地确定, 而系统的量子相干性确实仅对其电子计数统计特性有一个很小的影响. 需要指出的是, 共隧穿过程在这种情形下并不改变传输电子数目的内在统计特性, 例如, 电流累积矩的超泊松分布是否发生, 以及偏斜度和峭度 Fano 因子的数值是否发生符号转变, 见图 6.8 和图 6.9.

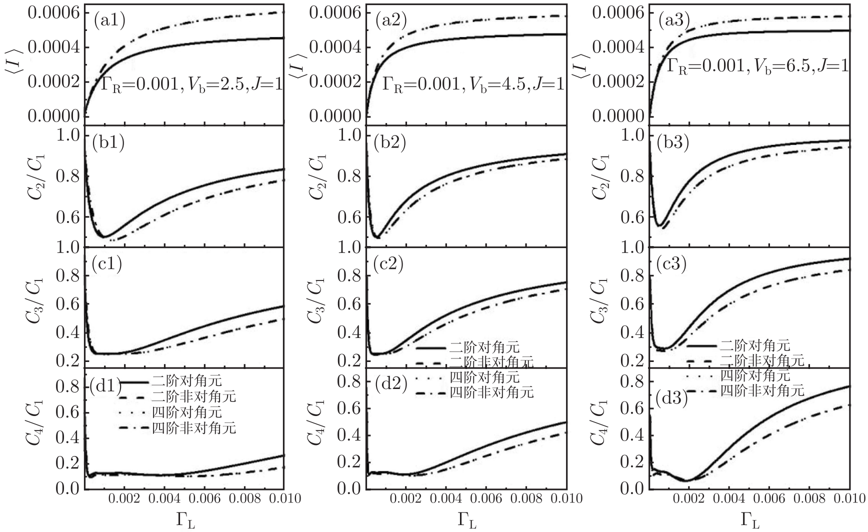


图 6.8 当 $k_BT = 0.1$ 和 $\Gamma_R = 0.001$ 时, T 型双量子点的电流前四阶累积矩, 即 (a1)～(a3) 平均电流 ($\langle I\rangle$)、(b1)～(b3) 散粒噪声 ($C_2/C_1$)、(c1)～(c3) 偏斜度 ($C_3/C_1$)、(d1)～(d3) 峭度 ($C_4/C_1$) 在不同偏压区域情形下随隧穿耦合强度 $\Gamma_L$ 的变化, 其中 $C_i$ 为电流的第 $i$ 阶零频累积矩

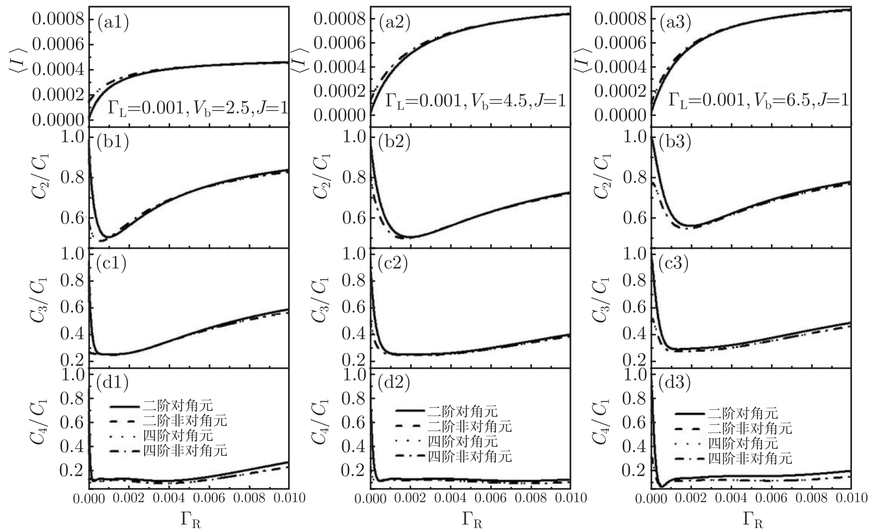


图 6.9 当 $k_BT = 0.1$ 和 $\Gamma_L = 0.001$ 时, T 型双量子点的电流前四阶累积矩, 即 (a1)～(a3) 平均电流 ($\langle I\rangle$)、(b1)～(b3) 散粒噪声 ($C_2/C_1$)、(c1)～(c3) 偏斜度 ($C_3/C_1$)、(d1)～(d3) 峭度 ($C_4/C_1$) 在不同偏压区域情形下随隧穿耦合强度 $\Gamma_R$ 的变化, 其中 $C_i$ 为电流的第 $i$ 阶零频累积矩

## 6.5 结 论

对于具有强量子相干性的开放 T 型双量子点系统, 在顺序隧穿占主导地位的偏压区域内, 共隧穿过程和量子相干性的相互竞争或相互作用决定了电流的散粒噪声、偏斜度和峭度是否为超泊松分布, 即 $C_i/C_1$ 的数值是否大于 1, 以及偏斜度和峭度的数值符号转变是否发生. 这些特性依赖于 T 型双量子点的温度、量子点与源极、漏极的不对称耦合以及相应隧穿耦合强度的大小. 但是, 在具有弱量子相干性的开放 T 型双量子点系统中, 共隧穿过程对其电子计数统计特性的影响比较小, 此特性同样依赖于量子点与源极、漏极的不对称耦合以及相应隧穿耦合强度的大小. 因此, 在具有强量子相干性的开放量子系统中, 即使在顺序隧穿占主导地位的偏压区域内, 共隧穿过程和量子相干性对其电子计数统计的影响也不能忽略.

### 参 考 文 献

[1] De Franceschi S, Sasaki S, Elzerman J M, et al. Electron cotunneling in a semiconductor quantum dot. Phys. Rev. Lett., 2001, 86: 878-881.

[2] Liu H W, Fujisawa T, Hayashi T, et al. Pauli spin blockade in cotunneling transport through a double quantum dot. Phys. Rev. B, 2005, 72: 161305(R).

[3] Schleser R, Ihn T, Ruh E, et al. Cotunneling-mediated transport through excited states in the Coulomb-blockade regime. Phys. Rev. Lett., 2005, 94: 206805.

[4] Sigrist M, Ihn T, Ensslin K, et al. Phase coherence in the inelastic cotunneling regime. Phys. Rev. Lett., 2006, 96: 036804.

[5] Jo M H, Grose J E, Baheti K, et al. Signatures of molecular magnetism in single-molecule transport spectroscopy. Nano Lett., 2006, 6: 2014-2020.

[6] Roch N, Vincent R, Elste F, et al. Cotunneling through a magnetic single-molecule transistor based on N@$C_{60}$. Phys. Rev. B, 2011, 83: 081407(R).

[7] Hartmann U, Wilhelm F K. Nonlinear cotunneling through an artificial molecule. Phys. Rev. B, 2003, 67: 161307(R).

[8] Golovach V N, Loss D. Transport through a double quantum dot in the sequential tunneling and cotunneling regimes. Phys. Rev. B, 2004, 69: 245327.

[9] Weymann I, Barnaś J. Effect of intrinsic spin relaxation on the spin-dependent cotunneling transport through quantum dots. Phys. Rev. B, 2006, 73: 205309.

[10] Elste F, Timm C. Cotunneling and nonequilibrium magnetization in magnetic molecular monolayers. Phys. Rev. B, 2007, 75: 195341.

[11] Misiorny M, Weymann I, Barnaś J. Spin effects in transport through single-molecule magnets in the sequential and cotunneling regimes. Phys. Rev. B, 2009, 79: 224420.

[12] Begemann G, Koller S, Grifoni M, et al. Inelastic cotunneling in quantum dots and molecules with weakly broken degeneracies. Phys. Rev. B, 2010, 82: 045316.

[13] Onac E, Balestro F, Trauzettel B, et al. Shot-noise detection in a carbon nanotube quantum dot. Phys. Rev. Lett., 2006, 96: 026803.

[14] Gustavsson S, Leturcq R, Simovič B, et al. Counting statistics and super-Poissonian noise in a quantum dot: Time-resolved measurements of electron transport. Phys. Rev. B, 2006, 74: 195305.

[15] Zhang Y, DiCarlo L, McClure D T, et al. Noise correlations in a Coulomb-blockaded quantum dot. Phys. Rev. Lett., 2007, 99: 036603.

[16] Zarchin O, Chung Y C, Heiblum M, et al. Electron bunching in transport through quantum dots in a high magnetic field. Phys. Rev. Lett., 2007, 98: 066801.

[17] Gustavsson S, Studer M, Leturcq R, et al. Detecting single-electron tunneling involving virtual processes in real time. Phys. Rev. B, 2008, 78: 155309.

[18] Okazaki Y, Sasaki S, Muraki K. Shot noise spectroscopy on a semiconductor quantum dot in the elastic and inelastic cotunneling regimes. Phys. Rev. B, 2013, 87: 041302(R).

[19] Thielmann A, Hettler M H, König J, et al. Cotunneling current and shot noise in quantum dots. Phys. Rev. Lett., 2005, 95: 146806.

[20] Weymann I. Effects of different geometries on the conductance, shot noise, and tunnel magnetoresistance of double quantum dots. Phys. Rev. B, 2008, 78: 045310.

[21] Weymann I, Barnaś J. Shot noise and tunnel magnetoresistance in multilevel quantum dots: Effects of cotunneling. Phys. Rev. B, 2008, 77: 075305.

[22] Aghassi J, Hettler M H, Schön G. Cotunneling assisted sequential tunneling in multilevel quantum dots. Appl. Phys. Lett., 2008, 92: 202101.

[23] Weymann I, Barnaś J. Eightfold shell-filling patterns in spin-dependent transport through double-wall carbon nanotube quantum dots. Phys. Rev. B, 2010, 82: 165450.

[24] Weymann I, Bułka B R, Barnaś J. Dark states in transport through triple quantum dots: The role of cotunneling. Phys. Rev. B, 2011, 83: 195302.

[25] Carmi A, Oreg Y. Enhanced shot noise in asymmetric interacting two-level systems. Phys. Rev. B, 2012, 85: 045325.

[26] Kaasbjerg K, Belzig W. Full counting statistics and shot noise of cotunneling in quantum dots and single-molecule transistors. Phys. Rev. B, 2015, 91: 235413.

[27] Wrześniewski K, Weymann I. Spin effects in transport through triangular quantum dot molecule in different geometrical configurations. Phys. Rev. B, 2015, 92: 045407.

[28] Sukhorukov E V, Burkard G, Loss D. Noise of a quantum dot system in the cotunneling regime. Phys. Rev. B, 2001, 63: 125315.

[29] Braggio A, König J, Fazio R. Full counting statistics in strongly interacting systems: Non-Markovian effects. Phys. Rev. Lett., 2006, 96: 026805.

[30] Utsumi Y, Golubev D S, Schön G. Full counting statistics for a single-electron transistor: Nonequilibrium effects at intermediate conductance. Phys. Rev. Lett., 2006, 96: 086803.

[31] Emary C. Counting statistics of cotunneling electrons. Phys. Rev. B, 2009, 80: 235306.

[32] Kießlich G, Schöll E, Brandes T, et al. Noise enhancement due to quantum coherence in coupled quantum dots. Phys. Rev. Lett., 2007, 99: 206602.

[33] Lindebaum S, Urban D, König J. Spin-induced charge correlations in transport through interacting quantum dots with ferromagnetic leads. Phys. Rev. B, 2009, 79: 245303.

[34] Urban D, König J. Tunable dynamical channel blockade in double-dot Aharonov-Bohm interferometers. Phys. Rev. B, 2009, 79: 165319.

[35] Xue H B. Full counting statistics as a probe of quantum coherence in a side-coupled double quantum dot system. Ann. Phys. (New York), 2013, 339: 208-217.

[36] Xue H B, Nie Y H, Chen J Z, et al. Probing the effective nuclear-spin magnetic field in a single quantum dot via full counting statistics. Ann. Phys. (New York), 2015, 354: 375-384.

[37] Xue H B, Nie Y H, Ren W. Negative differential conductance and super-Poissonian shot noise in a single quantum dot coupled to two noncollinear polarized ferromagnetic leads. Eur. Phys. J. B, 2015, 88: 76.

[38] Xue H B, Jiao H J, Liang J Q, et al. Non-Markovian full counting statistics in quantum dot molecules. Sci. Rep., 2015, 5: 8978.

[39] Marcos D, Emary C, Brandes T, et al. Non-Markovian effects in the quantum noise of interacting nanostructures. Phys. Rev. B, 2011, 83: 125426.

[40] Weymann I, Barnaś J, Krompiewski S. Transport through single-wall metallic carbon nanotubes in the cotunneling regime. Phys. Rev. B, 2008, 78: 035422.

[41] Luo J Y, Jiao H J, Shen Y, et al. Full counting statistics of level renormalization in electron transport through double quantum dots. J. Phys.: Condens. Matter, 2011, 23: 145301.

[42] Elzerman J M, Hanson R, Willems van Beveren L H, et al. Single-shot read-out of an individual electron spin in a quantum dot. Nature, 2004, 430: 431-435.

# 附　　录

## 附录 A　顺序隧穿中的 4 类积分

在本附录中, 给出基于量子主方程计算开放量子系统电子输运性质时, 用到的如下四个积分的计算过程:

$$\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{g_\alpha(\omega) f_\alpha(\omega)}{\mathrm{i}\eta+\omega-\Delta}, \tag{A.1}$$

$$\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{g_\alpha(\omega) f_\alpha(\omega)}{\mathrm{i}\eta-\omega-\Delta}, \tag{A.2}$$

$$\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{g_\alpha(\omega)\left[1-f_\alpha(\omega)\right]}{\mathrm{i}\eta+\omega-\Delta}, \tag{A.3}$$

$$\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{g_\alpha(\omega)\left[1-f_\alpha(\omega)\right]}{\mathrm{i}\eta-\omega-\Delta}, \tag{A.4}$$

其中

$$g_\alpha(\omega)=\frac{W^2}{\left(\omega-\mu_\alpha\right)^2+W^2}. \tag{A.5}$$

对于式 (A.1) 中的被积函数, 可将其重新表示为

$$\begin{aligned}
&\lim_{\eta\to 0^+} \frac{g_\alpha(\omega) f_\alpha(\omega)}{\mathrm{i}\eta+\omega-\Delta} \\
&=\lim_{\eta\to 0^+} \frac{g_\alpha(\omega) f_\alpha(\omega)(\omega-\Delta-\mathrm{i}\eta)}{(\omega-\Delta)^2+\eta^2} \\
&=\frac{g_\alpha(\omega) f_\alpha(\omega)}{\omega-\Delta}-\mathrm{i} g_\alpha(\omega) f_\alpha(\omega) \lim_{\eta\to 0^+} \frac{\eta}{(\omega-\Delta)^2+\eta^2} \\
&=\frac{g_\alpha(\omega) f_\alpha(\omega)}{\omega-\Delta}-\mathrm{i}\pi\delta(\omega-\Delta) g_\alpha(\omega) f_\alpha(\omega),
\end{aligned} \tag{A.6}$$

由式 (A.6) 代入式 (A.1) 可得

$$\begin{aligned}
&\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{g_\alpha(\omega) f_\alpha(\omega)}{\mathrm{i}\eta+\omega-\Delta} \\
&=P\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{g_\alpha(\omega) f_\alpha(\omega)}{\omega-\Delta}-\mathrm{i}\pi\int_{-\infty}^{\infty} \mathrm{d}\omega\, \delta(\omega-\Delta) g_\alpha(\omega) f_\alpha(\omega) \\
&=P\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{g_\alpha(\omega) f_\alpha(\omega)}{\omega-\Delta}-\mathrm{i}\pi g_\alpha(\Delta) f_\alpha(\Delta),
\end{aligned} \tag{A.7}$$

将式 (A.7) 右边第一项的主值积分展开为

$$\begin{aligned}&P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha(\omega)f_\alpha(\omega)}{\omega-\Delta}\\&=W^2P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{1}{1+\mathrm{e}^{\frac{\omega-\mu_\alpha}{k_\mathrm{B}T}}}\frac{1}{\omega-\Delta}\frac{1}{\omega-\mu_\alpha-\mathrm{i}W}\frac{1}{\omega-\mu_\alpha+\mathrm{i}W},\end{aligned}\tag{A.8}$$

为方便计算, 令 $\beta=1/k_\mathrm{B}T$, 且 $x=\beta(\omega-\mu_\alpha)$, 则式 (A.8) 可以写为

$$\begin{aligned}&P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha(\omega)f_\alpha(\omega)}{\omega-\Delta}\\&=(\beta W)^2P\int_{-\infty}^{\infty}\mathrm{d}x\frac{1}{1+\mathrm{e}^x}\frac{1}{x-x_1}\frac{1}{x-x_2}\frac{1}{x-x_3},\end{aligned}\tag{A.9}$$

其中

$$\begin{cases}x_1=\beta(\Delta-\mu_\alpha)\\x_2=\mathrm{i}\beta W\\x_3=-\mathrm{i}\beta W\end{cases}.\tag{A.10}$$

下面利用留数定理计算式 (A.9) 的主值积分, 并将其被积函数写为

$$f(z)=\frac{1}{1+\mathrm{e}^z}\frac{1}{z-x_1}\frac{1}{z-x_2}\frac{1}{z-x_3},\tag{A.11}$$

其奇点可以表示为

$$\begin{cases}z_{0,n}=\mathrm{i}(2n+1)\pi,\quad n=0,\pm1,\pm2,\cdots\\z_1=x_1\\z_2=x_2\\z_3=x_3\end{cases},\tag{A.12}$$

其中, $z_{0,n}$ 是虚轴上的一阶奇点, $z_1$ 是实轴上的一阶奇点, $z_2$ 是正虚轴上的一阶奇点, $z_3$ 是负虚轴上的一阶奇点. 积分路径选择为除奇点 $z_1$ 外的实轴部分和在上半平面内以原点为圆心、半径为 $R$ 的半圆组成的围道, 如图 A.1 所示. 由留数定理可知

$$\oint f(z)\mathrm{d}z=2\pi\mathrm{i}\sum_{n\geqslant0}\mathrm{Res}[f(z),z_{0,n}]+2\pi\mathrm{i}\mathrm{Res}[f(z),z_2],\tag{A.13}$$

其中

$$\begin{aligned}&\mathrm{Res}[f(z),z_{0,n}]\\&=\lim_{z\to z_{0,n}}(z-z_{0,n})\frac{1}{1+\mathrm{e}^z}\frac{1}{z-x_1}\frac{1}{z-x_2}\frac{1}{z-x_3}\end{aligned}$$

$$
\begin{aligned}
&= \frac{1}{\mathrm{e}^{z_{0,n}}} \frac{1}{z_{0,n}-x_1} \frac{1}{z_{0,n}-x_2} \frac{1}{z_{0,n}-x_3} \\
&= -\frac{1}{x_1-x_2} \frac{1}{x_1-x_3} \frac{1}{z_{0,n}-x_1} + \frac{1}{x_1-x_2} \frac{1}{x_1-x_3} \frac{1}{z_{0,n}-x_3} \\
&\quad + \frac{1}{x_1-x_2} \frac{1}{x_2-x_3} \frac{1}{z_{0,n}-x_2} - \frac{1}{x_1-x_2} \frac{1}{x_2-x_3} \frac{1}{z_{0,n}-x_3},
\end{aligned} \tag{A.14}
$$

$$
\begin{aligned}
&\mathrm{Res}\left[f(z), x_2\right] \\
&= \lim_{z\to x_2} (z-x_2) \frac{1}{1+\mathrm{e}^z} \frac{1}{z-x_1} \frac{1}{z-x_2} \frac{1}{z-x_3} \\
&= \lim_{z\to x_2} \frac{1}{1+\mathrm{e}^z} \frac{1}{z-x_1} \frac{1}{z-x_3} = \frac{1}{1+\mathrm{e}^{x_2}} \frac{1}{x_2-x_1} \frac{1}{x_2-x_3},
\end{aligned} \tag{A.15}
$$

将式 (A.14) 和式 (A.15) 代入式 (A.13) 可得

$$
\begin{aligned}
&\oint f(z)\mathrm{d}z \\
&= 2\pi\mathrm{i} \frac{1}{1+\mathrm{e}^{x_2}} \frac{1}{x_2-x_1} \frac{1}{x_2-x_3} \\
&\quad - 2\pi\mathrm{i} \frac{1}{x_1-x_2} \frac{1}{x_1-x_3} \sum_n \frac{1}{z_{0,n}-x_1} + 2\pi\mathrm{i} \frac{1}{x_1-x_2} \frac{1}{x_1-x_3} \sum_n \frac{1}{z_{0,n}-x_3} \\
&\quad + 2\pi\mathrm{i} \frac{1}{x_1-x_2} \frac{1}{x_2-x_3} \sum_n \frac{1}{z_{0,n}-x_2} - 2\pi\mathrm{i} \frac{1}{x_1-x_2} \frac{1}{x_2-x_3} \sum_n \frac{1}{z_{0,n}-x_3}.
\end{aligned} \tag{A.16}
$$

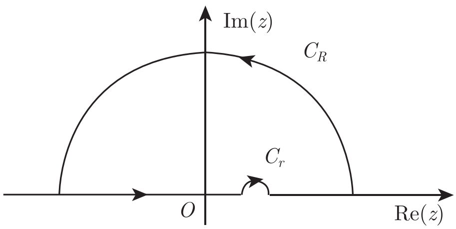


图 A.1　式 (A.13) 主值积分的围道

由于当 $|z| \to \infty$ 时, 积分

$$
\lim_{|z|\to\infty} zf(z) = \lim_{|z|\to\infty} z \frac{1}{1+\mathrm{e}^z} \frac{1}{z-x_1} \frac{1}{z-x_2} \frac{1}{z-x_3} = 0, \tag{A.17}
$$

因而有

$$
\int_{C_R} f(z)\,\mathrm{d}z = 0. \tag{A.18}
$$

此外, 积分

$$
\int_{C_r} f(z)\,\mathrm{d}z = -\mathrm{i}\pi \mathrm{Res}\left[f(z), x_1\right]
$$

$$
\begin{aligned}
&= -\mathrm{i}\pi \lim_{z \to x_1} (z - x_1) \frac{1}{1+\mathrm{e}^z} \frac{1}{z - x_1} \frac{1}{z - x_2} \frac{1}{z - x_3} \\
&= -\mathrm{i}\pi \frac{1}{1+\mathrm{e}^{x_1}} \frac{1}{x_1 - x_2} \frac{1}{x_1 - x_3}.
\end{aligned} \tag{A.19}
$$

当 $R \to \infty$, 且 $r \to 0$ 时, $f(z)$ 的主值积分可表示为

$$
\begin{aligned}
&P\int_{-\infty}^{\infty} \mathrm{d}x \frac{1}{1+\mathrm{e}^x} \frac{1}{x - x_1} \frac{1}{x - x_2} \frac{1}{x - x_3} \\
&= \oint f(z)\mathrm{d}z - \int_{C_R} f(z)\,\mathrm{d}z - \int_{C_r} f(z)\,\mathrm{d}z \\
&= 2\pi\mathrm{i} \frac{1}{1+\mathrm{e}^{x_2}} \frac{1}{x_2 - x_1} \frac{1}{x_2 - x_3} + \pi\mathrm{i} \frac{1}{1+\mathrm{e}^{x_1}} \frac{1}{x_1 - x_2} \frac{1}{x_1 - x_3} \\
&\quad - 2\pi\mathrm{i} \frac{1}{x_1 - x_2} \frac{1}{x_1 - x_3} \sum_{n=0}^{\infty} \frac{1}{z_{0,n} - x_1} + 2\pi\mathrm{i} \frac{1}{x_1 - x_2} \frac{1}{x_1 - x_3} \sum_{n=0}^{\infty} \frac{1}{z_{0,n} - x_3} \\
&\quad + 2\pi\mathrm{i} \frac{1}{x_1 - x_2} \frac{1}{x_2 - x_3} \sum_{n=0}^{\infty} \frac{1}{z_{0,n} - x_2} - 2\pi\mathrm{i} \frac{1}{x_1 - x_2} \frac{1}{x_2 - x_3} \sum_{n=0}^{\infty} \frac{1}{z_{0,n} - x_3},
\end{aligned} \tag{A.20}
$$

由双伽马函数的性质 [1]

$$
\Psi(z) = \lim_{n \to \infty} \left( \ln n - \sum_{k=0}^{\infty} \frac{1}{k + z} \right), \tag{A.21}
$$

可将式 (A.20) 简化为

$$
\begin{aligned}
&P\int_{-\infty}^{\infty} \mathrm{d}x \frac{1}{1+\mathrm{e}^x} \frac{1}{x - x_1} \frac{1}{x - x_2} \frac{1}{x - x_3} \\
&= 2\pi\mathrm{i} \frac{1}{1+\mathrm{e}^{x_2}} \frac{1}{x_2 - x_1} \frac{1}{x_2 - x_3} + \pi\mathrm{i} \frac{1}{1+\mathrm{e}^{x_1}} \frac{1}{x_1 - x_2} \frac{1}{x_1 - x_3} \\
&\quad + \frac{1}{x_1 - x_2} \frac{1}{x_1 - x_3} \Psi\left(\frac{1}{2} + \mathrm{i}\frac{x_1}{2\pi}\right) - \frac{1}{x_1 - x_2} \frac{1}{x_1 - x_3} \Psi\left(\frac{1}{2} + \mathrm{i}\frac{x_3}{2\pi}\right) \\
&\quad - \frac{1}{x_1 - x_2} \frac{1}{x_2 - x_3} \Psi\left(\frac{1}{2} + \mathrm{i}\frac{x_2}{2\pi}\right) + \frac{1}{x_1 - x_2} \frac{1}{x_2 - x_3} \Psi\left(\frac{1}{2} + \mathrm{i}\frac{x_3}{2\pi}\right),
\end{aligned} \tag{A.22}
$$

利用双伽马函数的性质 [1]

$$
\Psi(z) = \Psi(1 - z) - \pi \cot(\pi z), \tag{A.23}
$$

可得

$$
\Psi\left(\frac{1}{2} + \mathrm{i}\frac{x_1}{2\pi}\right) = \Psi\left(\frac{1}{2} - \mathrm{i}\frac{x_1}{2\pi}\right) - \mathrm{i}\pi \tanh\left(-\frac{x_1}{2}\right), \tag{A.24}
$$

$$
\Psi\left(\frac{1}{2} + \mathrm{i}\frac{x_2}{2\pi}\right) = \Psi\left(\frac{1}{2} - \mathrm{i}\frac{x_2}{2\pi}\right) + \pi \tan\left(\mathrm{i}\frac{x_2}{2}\right), \tag{A.25}
$$

考虑到 $[\Psi(z)]^* = \Psi(z^*)$, 因此有

$$\Psi\left(\frac{1}{2}+\mathrm{i}\frac{x_1}{2\pi}\right) = \mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{x_1}{2\pi}\right) - \frac{\mathrm{i}\pi}{2}\tanh\left(-\frac{x_1}{2}\right), \tag{A.26}$$

将式 (A.25) 和式 (A.26) 代入式 (A.22), 并考虑到 $x_2 = -x_3 = \mathrm{i}\beta W$, 可得

$$\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}x\frac{1}{1+\mathrm{e}^x}\frac{1}{x-x_1}\frac{1}{x-x_2}\frac{1}{x-x_3}\\
=&\pi\mathrm{i}\frac{1}{x_1-x_2}\frac{1}{x_1+x_2}\left[\frac{1}{1+\mathrm{e}^{x_1}}-\frac{1}{2}\tanh\left(-\frac{x_1}{2}\right)\right]\\
&+\frac{1}{x_1-x_2}\frac{1}{x_1+x_2}\left[\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{x_1}{2\pi}\right)-\Psi\left(\frac{1}{2}-\mathrm{i}\frac{x_2}{2\pi}\right)\right]\\
&-\frac{1}{x_1-x_2}\frac{1}{2x_2}\left[\frac{2\pi\mathrm{i}}{1+\mathrm{e}^{x_2}}+\pi\tan\left(\mathrm{i}\frac{x_2}{2}\right)\right],
\end{aligned}\tag{A.27}$$

由于式 (A.27) 中

$$\frac{1}{1+\mathrm{e}^{x_1}}-\frac{1}{2}\tanh\left(-\frac{x_1}{2}\right)=\frac{1}{2}, \tag{A.28}$$

$$\frac{2\pi\mathrm{i}}{1+\mathrm{e}^{x_2}}+\pi\tan\left(\mathrm{i}\frac{x_2}{2}\right)=\mathrm{i}\pi, \tag{A.29}$$

因而, 式 (A.27) 可进一步简化为

$$\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}x\frac{1}{1+\mathrm{e}^x}\frac{1}{x-x_1}\frac{1}{x-x_2}\frac{1}{x-x_3}\\
=&\frac{\pi\mathrm{i}}{2}\frac{1}{x_1-x_2}\frac{1}{x_1+x_2}-\pi\mathrm{i}\frac{1}{x_1-x_2}\frac{1}{2x_2}\\
&+\frac{1}{x_1-x_2}\frac{1}{x_1+x_2}\left[\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{x_1}{2\pi}\right)-\Psi\left(\frac{1}{2}-\mathrm{i}\frac{x_2}{2\pi}\right)\right],
\end{aligned}\tag{A.30}$$

将式 (A.10) 代入式 (A.30) 可得

$$\begin{aligned}
&(\beta W)^2 P\int_{-\infty}^{\infty}\mathrm{d}x\frac{1}{1+\mathrm{e}^x}\frac{1}{x-x_1}\frac{1}{x-x_2}\frac{1}{x-x_3}\\
=&g_\alpha(\Delta)\left[\frac{\pi\mathrm{i}}{2}-\frac{\pi}{2}\frac{(\Delta-\mu_\alpha)+\mathrm{i}W}{W}+\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{\Delta-\mu_\alpha}{2\pi k_{\mathrm{B}}T}\right)-\Psi\left(\frac{1}{2}+\frac{W}{2\pi k_{\mathrm{B}}T}\right)\right]\\
=&g_\alpha(\Delta)\left[\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{\Delta-\mu_\alpha}{2\pi k_{\mathrm{B}}T}\right)-\Psi\left(\frac{1}{2}+\frac{W}{2\pi k_{\mathrm{B}}T}\right)-\frac{\pi}{2}\frac{\Delta-\mu_\alpha}{W}\right],
\end{aligned}\tag{A.31}$$

将式 (A.31) 代入式 (A.9) 可得

$$P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha(\omega)f_\alpha(\omega)}{\omega-\Delta}$$

$$= g_\alpha(\Delta)\left[\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{\Delta-\mu_\alpha}{2\pi k_\mathrm{B}T}\right)-\Psi\left(\frac{1}{2}+\frac{W}{2\pi k_\mathrm{B}T}\right)-\frac{\pi}{2}\frac{\Delta-\mu_\alpha}{W}\right], \quad \text{(A.32)}$$

继续将式 (A.32) 代入式 (A.7) 可得

$$\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha(\omega)f_\alpha(\omega)}{\mathrm{i}\eta+\omega-\Delta}$$
$$= g_\alpha(\Delta)\left[\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{\Delta-\mu_\alpha}{2\pi k_\mathrm{B}T}\right)-\Psi\left(\frac{1}{2}+\frac{W}{2\pi k_\mathrm{B}T}\right)-\frac{\pi}{2}\frac{\Delta-\mu_\alpha}{W}-\mathrm{i}\pi f_\alpha(\Delta)\right], \quad \text{(A.33)}$$

在宽带近似下, 即 $W \gg \mathrm{Max}\{\varepsilon,\mu_\alpha,k_\mathrm{B}T,\Delta\}$, 式 (A.32) 和式 (A.33) 可进一步简化为

$$P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha(\omega)f_\alpha(\omega)}{\omega-\Delta}=\left[\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{\Delta-\mu_\alpha}{2\pi k_\mathrm{B}T}\right)-\ln\frac{W}{2\pi k_\mathrm{B}T}\right], \quad \text{(A.34)}$$

$$\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha(\omega)f_\alpha(\omega)}{\mathrm{i}\eta+\omega-\Delta}=\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{\Delta-\mu_\alpha}{2\pi k_\mathrm{B}T}\right)-\ln\frac{W}{2\pi k_\mathrm{B}T}-\mathrm{i}\pi f_\alpha(\Delta), \quad \text{(A.35)}$$

其中上面两式简化中用到了双伽马函数的性质 [1]

$$\lim_{n\to\infty}[\Psi(z+n)-\ln n]=0. \quad \text{(A.36)}$$

下面计算式 (A.2) 积分, 由于其被积函数可以表示为

$$\lim_{\eta\to0^+}\frac{g_\alpha(\omega)f_\alpha(\omega)}{\mathrm{i}\eta-\omega-\Delta}$$
$$=\lim_{\eta\to0^+}\frac{g_\alpha(\omega)f_\alpha(\omega)(-\omega-\Delta-\mathrm{i}\eta)}{(\omega+\Delta)^2+\eta^2}$$
$$=-\frac{g_\alpha(\omega)f_\alpha(\omega)}{\omega+\Delta}-\mathrm{i}g_\alpha(\omega)f_\alpha(\omega)\lim_{\eta\to0^+}\frac{\eta}{(\omega+\Delta)^2+\eta^2}$$
$$=-\frac{g_\alpha(\omega)f_\alpha(\omega)}{\omega+\Delta}-\mathrm{i}\pi\delta(\omega+\Delta)g_\alpha(\omega)f_\alpha(\omega), \quad \text{(A.37)}$$

因此, 式 (A.2) 可以重新表示为

$$\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha(\omega)f_\alpha(\omega)}{\mathrm{i}\eta-\omega-\Delta}=-P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha(\omega)f_\alpha(\omega)}{\omega+\Delta}-\mathrm{i}\pi g_\alpha(-\Delta)f_\alpha(-\Delta). \quad \text{(A.38)}$$

将式 (A.32) 中的 $\Delta\to-\Delta$ 可得

$$P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha(\omega)f_\alpha(\omega)}{\omega+\Delta}$$
$$= g_\alpha(-\Delta)\left[\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{-\Delta-\mu_\alpha}{2\pi k_\mathrm{B}T}\right)-\Psi\left(\frac{1}{2}+\frac{W}{2\pi k_\mathrm{B}T}\right)-\frac{\pi}{2}\frac{-\Delta-\mu_\alpha}{W}\right], \quad \text{(A.39)}$$

将式 (A.39) 代入式 (A.38) 可得

$$
\begin{aligned}
&\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha\left(\omega\right)f_\alpha\left(\omega\right)}{\mathrm{i}\eta-\omega-\Delta}\\
&=g_\alpha\left(-\Delta\right)\\
&\quad\times\left[-\mathrm{Re}\Psi\left(\frac{1}{2}-\mathrm{i}\frac{\Delta+\mu_\alpha}{2\pi k_\mathrm{B}T}\right)+\Psi\left(\frac{1}{2}+\frac{W}{2\pi k_\mathrm{B}T}\right)-\frac{\pi}{2}\frac{\Delta+\mu_\alpha}{W}-\mathrm{i}\pi f_\alpha\left(-\Delta\right)\right],
\end{aligned}
\tag{A.40}
$$

在宽带近似下, 即 $W\gg\mathrm{Max}\left\{\varepsilon,\mu_\alpha,k_\mathrm{B}T,\Delta\right\}$, 并考虑到式 (A.36), 式 (A.39) 和式 (A.40) 可进一步简化为

$$
P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha\left(\omega\right)f_\alpha\left(\omega\right)}{\omega+\Delta}=\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{-\Delta-\mu_\alpha}{2\pi k_\mathrm{B}T}\right)-\ln\frac{W}{2\pi k_\mathrm{B}T},\tag{A.41}
$$

$$
\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha\left(\omega\right)f_\alpha\left(\omega\right)}{\mathrm{i}\eta-\omega-\Delta}=-\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{-\Delta-\mu_\alpha}{2\pi k_\mathrm{B}T}\right)+\ln\frac{W}{2\pi k_\mathrm{B}T}-\mathrm{i}\pi f_\alpha\left(-\Delta\right).\tag{A.42}
$$

现在, 计算式 (A.3) 和式 (A.4) 的积分. 为此, 首先计算下面的主值积分:

$$
\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha\left(\omega\right)}{\omega-\Delta}\\
&=W^2P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{1}{\omega-\Delta}\frac{1}{\omega-\mu_\alpha-\mathrm{i}W}\frac{1}{\omega-\mu_\alpha+\mathrm{i}W}\\
&=W^2P\int_{-\infty}^{\infty}\mathrm{d}x\frac{1}{x-x_1}\frac{1}{x-x_2}\frac{1}{x-x_3},
\end{aligned}
\tag{A.43}
$$

其中

$$
\left\{\begin{aligned}
&x_1=\Delta\\
&x_2=\mu_\alpha+\mathrm{i}W\\
&x_3=\mu_\alpha-\mathrm{i}W
\end{aligned}\right..\tag{A.44}
$$

下面利用留数定理计算式 (A.43) 的主值积分, 并将其被积函数写为

$$
f\left(z\right)=\frac{1}{z-x_1}\frac{1}{z-x_2}\frac{1}{z-x_3},\tag{A.45}
$$

其奇点可以表示为

$$
\left\{\begin{aligned}
&z_1=x_1\\
&z_2=x_2\\
&z_3=x_3
\end{aligned}\right.,\tag{A.46}
$$

其中, $z_1$ 是实轴上的一阶奇点, $z_2$ 是上半平面的一阶奇点, $z_3$ 是下半平面的一阶奇点. 积分路径选择如图 A.1 所示. 由留数定理可知

$$
\oint f(z)\mathrm{d}z=2\pi\mathrm{i}\mathrm{Res}\left[f\left(z\right),x_2\right]=2\pi\mathrm{i}\lim_{z\to x_2}\left(z-x_2\right)f\left(z\right)
$$

$$
= 2\pi \mathrm{i} \lim_{z \to x_2} (z - x_2) \frac{1}{z - x_1} \frac{1}{z - x_2} \frac{1}{z - x_3} = 2\pi \mathrm{i} \frac{1}{x_2 - x_1} \frac{1}{x_2 - x_3}, \quad (A.47)
$$

由于当 $|z| \to \infty$ 时, 积分

$$
\lim_{|z| \to \infty} z f(z) = \lim_{|z| \to \infty} z \frac{1}{z - x_1} \frac{1}{z - x_2} \frac{1}{z - x_3} = 0, \quad (A.48)
$$

因而有

$$
\int_{C_R} f(z) \, \mathrm{d}z = 0. \quad (A.49)
$$

此外, 积分

$$
\begin{aligned}
\int_{C_r} f(z) \, \mathrm{d}z &= -\mathrm{i}\pi \mathrm{Res}\left[f(z), x_1\right] \\
&= -\mathrm{i}\pi \lim_{z \to x_1} (z - x_1) \frac{1}{z - x_1} \frac{1}{z - x_2} \frac{1}{z - x_3} \\
&= -\mathrm{i}\pi \frac{1}{x_1 - x_2} \frac{1}{x_1 - x_3}.
\end{aligned} \quad (A.50)
$$

当 $R \to \infty$ 且 $r \to 0$ 时, $f(z)$ 的主值积分可表示为

$$
\begin{aligned}
& P \int_{-\infty}^{\infty} \mathrm{d}x \frac{1}{x - x_1} \frac{1}{x - x_2} \frac{1}{x - x_3} \\
&= \oint f(z) \mathrm{d}z - \int_{C_R} f(z) \, \mathrm{d}z - \int_{C_r} f(z) \, \mathrm{d}z \\
&= 2\pi \mathrm{i} \frac{1}{x_2 - x_1} \frac{1}{x_2 - x_3} + \pi \mathrm{i} \frac{1}{x_1 - x_2} \frac{1}{x_1 - x_3},
\end{aligned} \quad (A.51)
$$

将式 (A.44) 代入式 (A.51) 可得

$$
\begin{aligned}
& W^2 P \int_{-\infty}^{\infty} \mathrm{d}x \frac{1}{x - x_1} \frac{1}{x - x_2} \frac{1}{x - x_3} \\
&= -\frac{W^2 2\pi \mathrm{i}}{2\mathrm{i}W (\Delta - \mu_\alpha - \mathrm{i}W)} + \frac{\pi \mathrm{i} W^2}{(\Delta - \mu_\alpha - \mathrm{i}W)(\Delta - \mu_\alpha + \mathrm{i}W)} \\
&= -\frac{(\Delta - \mu_\alpha)\pi + \mathrm{i}\pi W}{W} \frac{W^2}{(\Delta - \mu_\alpha)^2 + W^2} - \frac{W^2}{(\Delta - \mu_\alpha)^2 + W^2} + \frac{\pi \mathrm{i} W^2}{(\Delta - \mu_\alpha)^2 + W^2} \\
&= -\pi \frac{\Delta - \mu_\alpha}{W} g_\alpha(\Delta),
\end{aligned} \quad (A.52)
$$

继续将式 (A.52) 代入式 (A.43) 可得

$$
P \int_{-\infty}^{\infty} \mathrm{d}\omega \frac{g_\alpha(\omega)}{\omega - \Delta} = -\pi \frac{\Delta - \mu_\alpha}{W} g_\alpha(\Delta), \quad (A.53)
$$

由式 (A.53) 和式 (A.32) 可知

$$
\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha(\omega)[1-f_\alpha(\omega)]}{\omega-\Delta}\\
&=g_\alpha(\Delta)\left[-\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{\Delta-\mu_\alpha}{2\pi k_\mathrm{B}T}\right)+\Psi\left(\frac{1}{2}+\frac{W}{2\pi k_\mathrm{B}T}\right)-\frac{\pi}{2}\frac{\Delta-\mu_\alpha}{W}\right],
\end{aligned}\tag{A.54}
$$

对于式 (A.3) 中的被积函数, 可将其重新表示为

$$
\begin{aligned}
&\lim_{\eta\to0^+}\frac{g_\alpha(\omega)[1-f_\alpha(\omega)]}{\mathrm{i}\eta+\omega-\Delta}\\
&=\frac{g_\alpha(\omega)[1-f_\alpha(\omega)]}{\omega-\Delta}-\mathrm{i}\pi\delta(\omega-\Delta)\,g_\alpha(\omega)[1-f_\alpha(\omega)],
\end{aligned}\tag{A.55}
$$

因而, 式 (A.3) 的积分为

$$
\begin{aligned}
&\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha(\omega)[1-f_\alpha(\omega)]}{\mathrm{i}\eta+\omega-\Delta}\\
&=g_\alpha(\Delta)\\
&\quad\times\left\{-\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{\Delta-\mu_\alpha}{2\pi k_\mathrm{B}T}\right)+\Psi\left(\frac{1}{2}+\frac{W}{2\pi k_\mathrm{B}T}\right)-\frac{\pi}{2}\frac{\Delta-\mu_\alpha}{W}-\mathrm{i}\pi[1-f_\alpha(\Delta)]\right\},
\end{aligned}\tag{A.56}
$$

在宽带近似下, 即 $W\gg\max\{\varepsilon,\mu_\alpha,k_\mathrm{B}T,\Delta\}$, 并考虑到式 (A.36), 式 (A.54) 和式 (A.56) 可进一步简化为

$$
P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha(\omega)[1-f_\alpha(\omega)]}{\omega-\Delta}=-\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{\Delta-\mu_\alpha}{2\pi k_\mathrm{B}T}\right)+\ln\frac{W}{2\pi k_\mathrm{B}T},\tag{A.57}
$$

$$
\begin{aligned}
&\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha(\omega)[1-f_\alpha(\omega)]}{\mathrm{i}\eta+\omega-\Delta}\\
&=-\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{\Delta-\mu_\alpha}{2\pi k_\mathrm{B}T}\right)+\ln\frac{W}{2\pi k_\mathrm{B}T}-\mathrm{i}\pi[1-f_\alpha(\Delta)].
\end{aligned}\tag{A.58}
$$

将式 (A.54) 中的 $\Delta\to-\Delta$ 可得

$$
\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha(\omega)[1-f_\alpha(\omega)]}{\omega+\Delta}\\
&=g_\alpha(-\Delta)\left[-\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{-\Delta-\mu_\alpha}{2\pi k_\mathrm{B}T}\right)+\Psi\left(\frac{1}{2}+\frac{W}{2\pi k_\mathrm{B}T}\right)-\frac{\pi}{2}\frac{-\Delta-\mu_\alpha}{W}\right],
\end{aligned}\tag{A.59}
$$

将式 (A.59) 代入式 (A.4) 可得

$$
\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha(\omega)[1-f_\alpha(\omega)]}{\mathrm{i}\eta-\omega-\Delta}
$$

$$
\begin{aligned}
&= -P\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{g_\alpha(\omega)[1-f_\alpha(\omega)]}{\omega+\Delta} - \mathrm{i}\pi g_\alpha(-\Delta)[1-f_\alpha(-\Delta)] \\
&= g_\alpha(-\Delta) \\
&\quad \times \left[\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{-\Delta-\mu_\alpha}{2\pi k_\mathrm{B}T}\right) - \Psi\left(\frac{1}{2}+\frac{W}{2\pi k_\mathrm{B}T}\right) + \frac{\pi}{2}\frac{-\Delta-\mu_\alpha}{W} - \mathrm{i}\pi[1-f_\alpha(-\Delta)]\right].
\end{aligned} \tag{A.60}
$$

在宽带近似下, 即 $W \gg \max\{\varepsilon, \mu_\alpha, k_\mathrm{B}T, \Delta\}$, 并考虑到式 (A.36), 式 (A.59) 和式 (A.60) 可进一步简化为

$$
P\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{g_\alpha(\omega)[1-f_\alpha(\omega)]}{\omega+\Delta} = -\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{-\Delta-\mu_\alpha}{2\pi k_\mathrm{B}T}\right) + \ln\frac{W}{2\pi k_\mathrm{B}T}, \tag{A.61}
$$

$$
\begin{aligned}
&\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{g_\alpha(\omega)[1-f_\alpha(\omega)]}{\mathrm{i}\eta-\omega-\Delta} \\
&= \mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{-\Delta-\mu_\alpha}{2\pi k_\mathrm{B}T}\right) - \ln\frac{W}{2\pi k_\mathrm{B}T} - \mathrm{i}\pi[1-f_\alpha(-\Delta)].
\end{aligned} \tag{A.62}
$$

# 附录 B　顺序隧穿中的 4 类矩阵元

在本附录中, 给出式 (2.87)~ 式 (2.90) 中四个矩阵元

$$\langle m|\left[f_\alpha^{(\pm)}(L_\mathrm{QS})\,d_{\mu'}\right]\rho_\mathrm{QS}(t)\,|n\rangle, \tag{B.1}$$

$$\langle m|\left[f_\alpha^{(\pm)}(L_\mathrm{QS})\,d_{\mu'}^\dagger\right]\rho_\mathrm{QS}(t)\,|n\rangle, \tag{B.2}$$

$$\langle m|\,\rho_\mathrm{QS}(t)\left[f_\alpha^{(\pm)}(L_\mathrm{QS})\,d_{\mu'}\right]|n\rangle, \tag{B.3}$$

$$\langle m|\,\rho_\mathrm{QS}(t)\left[f_\alpha^{(\pm)}(L_\mathrm{QS})\,d_{\mu'}^\dagger\right]|n\rangle, \tag{B.4}$$

的具体表达式. 这里, 记量子系统哈密顿量 $H_\mathrm{QS}$ 的本征值和本征态满足

$$H_\mathrm{QS}\,|n\rangle = \varepsilon_n\,|n\rangle. \tag{B.5}$$

对于 $\langle m|\left[(L_\mathrm{QS})^1\,d_{\mu'}\right]\rho_\mathrm{QS}(t)\,|n\rangle$, 其可以表示为

$$
\begin{aligned}
\langle m|\,(L_\mathrm{QS}d_{\mu'})\,\rho_\mathrm{QS}(t)\,|n\rangle &= \langle m|\,(H_\mathrm{QS}d_{\mu'} - d_{\mu'}H_\mathrm{QS})\,\rho_\mathrm{QS}(t)\,|n\rangle \\
&= \varepsilon_m\,\langle m|\,d_{\mu'}\rho_\mathrm{QS}(t)\,|n\rangle - \langle m|\,d_{\mu'}H_\mathrm{QS}\rho_\mathrm{QS}(t)\,|n\rangle,
\end{aligned} \tag{B.6}
$$

若记 $\langle m|\,d_{\mu'} = \langle m'|$, 则式 (B.6) 可写为

$$\langle m|\,(L_\mathrm{QS}d_{\mu'})\,\rho_\mathrm{QS}(t)\,|n\rangle$$

$$
\begin{aligned}
&= \varepsilon_m \langle m'| \rho_{\mathrm{QS}}(t) |n\rangle - \langle m'| H_{\mathrm{QS}} \rho_{\mathrm{QS}}(t) |n\rangle \\
&= \varepsilon_m \langle m'| \rho_{\mathrm{QS}}(t) |n\rangle - \varepsilon_{m'} \langle m'| \rho_{\mathrm{QS}}(t) |n\rangle = (\varepsilon_m - \varepsilon_{m'}) \langle m'| \rho_{\mathrm{QS}}(t) |n\rangle .
\end{aligned} \tag{B.7}
$$

对于 $\langle m| [(L_{\mathrm{QS}})^2 d_{\mu'}]\rho_{\mathrm{QS}}(t) |n\rangle$, 其可以表示为

$$
\begin{aligned}
&\langle m| [(L_{\mathrm{QS}})^2 d_{\mu'}]\rho_{\mathrm{QS}}(t) |n\rangle \\
&= \langle m| [H_{\mathrm{QS}} (H_{\mathrm{QS}} d_{\mu'} - d_{\mu'} H_{\mathrm{QS}}) - (H_{\mathrm{QS}} d_{\mu'} - d_{\mu'} H_{\mathrm{QS}}) H_{\mathrm{QS}}] \rho_{\mathrm{QS}}(t) |n\rangle \\
&= \varepsilon_m \langle m| (H_{\mathrm{QS}} d_{\mu'} - d_{\mu'} H_{\mathrm{QS}}) \rho_{\mathrm{QS}}(t) |n\rangle \\
&\quad - \varepsilon_m \langle m| d_{\mu'} H_{\mathrm{QS}} \rho_{\mathrm{QS}}(t) |n\rangle + \langle m'| H_{\mathrm{QS}} H_{\mathrm{QS}} \rho_{\mathrm{QS}}(t) |n\rangle \\
&= \varepsilon_m (\varepsilon_m - \varepsilon_{m'}) \langle m'| \rho_{\mathrm{QS}}(t) |n\rangle - \varepsilon_m \varepsilon_{m'} \langle m'| \rho_{\mathrm{QS}}(t) |n\rangle + (\varepsilon_{m'})^2 \langle m'| \rho_{\mathrm{QS}}(t) |n\rangle \\
&= (\varepsilon_m - \varepsilon_{m'})^2 \langle m'| \rho_{\mathrm{QS}}(t) |n\rangle ,
\end{aligned} \tag{B.8}
$$

对于 $\langle m| [(L_{\mathrm{QS}})^3 d_{\mu'}]\rho_{\mathrm{QS}}(t) |n\rangle$, 其可以表示为

$$
\begin{aligned}
&\langle m| [(L_{\mathrm{QS}})^3 d_{\mu'}]\rho_{\mathrm{QS}}(t) |n\rangle \\
&= \langle m| H_{\mathrm{QS}} H_{\mathrm{QS}} (H_{\mathrm{QS}} d_{\mu'} - d_{\mu'} H_{\mathrm{QS}}) \rho_{\mathrm{QS}}(t) |n\rangle \\
&\quad - 2 \langle m| H_{\mathrm{QS}} (H_{\mathrm{QS}} d_{\mu'} - d_{\mu'} H_{\mathrm{QS}}) H_{\mathrm{QS}} \rho_{\mathrm{QS}}(t) |n\rangle \\
&\quad + \langle m| (H_{\mathrm{QS}} d_{\mu'} - d_{\mu'} H_{\mathrm{QS}}) H_{\mathrm{QS}} H_{\mathrm{QS}} \rho_{\mathrm{QS}}(t) |n\rangle \\
&= (\varepsilon_m)^2 \langle m| (H_{\mathrm{QS}} d_{\mu'} - d_{\mu'} H_{\mathrm{QS}}) \rho_{\mathrm{QS}}(t) |n\rangle \\
&\quad - 2\varepsilon_m \langle m| H_{\mathrm{QS}} d_{\mu'} H_{\mathrm{QS}} \rho_{\mathrm{QS}}(t) |n\rangle + 2\varepsilon_m \langle m| d_{\mu'} H_{\mathrm{QS}} H_{\mathrm{QS}} \rho_{\mathrm{QS}}(t) |n\rangle \\
&\quad + \varepsilon_m \langle m| d_{\mu'} H_{\mathrm{QS}} H_{\mathrm{QS}} \rho_{\mathrm{QS}}(t) |n\rangle - \langle m'| H_{\mathrm{QS}} H_{\mathrm{QS}} H_{\mathrm{QS}} \rho_{\mathrm{QS}}(t) |n\rangle \\
&= (\varepsilon_m)^2 (\varepsilon_m - \varepsilon_{m'}) \langle m'| \rho_{\mathrm{QS}}(t) |n\rangle \\
&\quad - 2 (\varepsilon_m)^2 \langle m| d_{\mu'} H_{\mathrm{QS}} \rho_{\mathrm{QS}}(t) |n\rangle + 2\varepsilon_m \langle m'| H_{\mathrm{QS}} H_{\mathrm{QS}} \rho_{\mathrm{QS}}(t) |n\rangle \\
&\quad + \varepsilon_m \langle m'| H_{\mathrm{QS}} H_{\mathrm{QS}} \rho_{\mathrm{QS}}(t) |n\rangle - (\varepsilon_{m'})^3 \langle m'| \rho_{\mathrm{QS}}(t) |n\rangle \\
&= (\varepsilon_m)^2 (\varepsilon_m - \varepsilon_{m'}) \langle m'| \rho_{\mathrm{QS}}(t) |n\rangle - 2 (\varepsilon_m)^2 \varepsilon_{m'} \langle m'| \rho_{\mathrm{QS}}(t) |n\rangle \\
&\quad + 2\varepsilon_m (\varepsilon_{m'})^2 \langle m'| \rho_{\mathrm{QS}}(t) |n\rangle + \varepsilon_m (\varepsilon_{m'})^2 \langle m'| \rho_{\mathrm{QS}}(t) |n\rangle \\
&\quad - (\varepsilon_{m'})^3 \langle m'| \rho_{\mathrm{QS}}(t) |n\rangle ,
\end{aligned} \tag{B.9}
$$

即

$$
\langle m| [(L_{\mathrm{QS}})^3 d_{\mu'}]\rho_{\mathrm{QS}}(t) |n\rangle = (\varepsilon_m - \varepsilon_{m'})^3 \langle m'| \rho_{\mathrm{QS}}(t) |n\rangle . \tag{B.10}
$$

同理, 可以证明

$$
\langle m| [(L_{\mathrm{QS}})^k d_{\mu'}]\rho_{\mathrm{QS}}(t) |n\rangle = (\varepsilon_m - \varepsilon_{m'})^k \langle m'| \rho_{\mathrm{QS}}(t) |n\rangle . \tag{B.11}
$$

因此, 式 (B.1) 可以写为

$$\langle m|\,[f_\alpha^{(\pm)}\,(L_{\mathrm{QS}})\,d_{\mu'}]\rho_{\mathrm{QS}}\,(t)\,|n\rangle = f_\alpha^{(\pm)}\,(\varepsilon_m-\varepsilon_{m'})\,\langle m'|\,\rho_{\mathrm{QS}}\,(t)\,|n\rangle\,, \tag{B.12}$$

其中

$$\langle m|\,d_{\mu'} = \langle m'|\,. \tag{B.13}$$

同理, 式 (B.2) 可以写为

$$\langle m|\,[f_\alpha^{(\pm)}\,(L_{\mathrm{QS}})\,d_{\mu'}^\dagger]\rho_{\mathrm{QS}}\,(t)\,|n\rangle = f_\alpha^{(\pm)}\,(\varepsilon_m-\varepsilon_{m''})\,\langle m''|\,\rho_{\mathrm{QS}}\,(t)\,|n\rangle\,. \tag{B.14}$$

其中

$$\langle m|\,d_{\mu'}^\dagger = \langle m''|\,. \tag{B.15}$$

下面计算式 (B.3) 和式 (B.4) 的矩阵元. 对于 $\langle m|\,\rho_{\mathrm{QS}}\,(t)\,[(L_{\mathrm{QS}})^1\,d_{\mu'}]\,|n\rangle$, 其可以表示为

$$\begin{aligned}
&\langle m|\,\rho_{\mathrm{QS}}\,(t)\,(L_{\mathrm{QS}}d_{\mu'})\,|n\rangle\\
&=\langle m|\,\rho_{\mathrm{QS}}\,(t)\,(H_{\mathrm{QS}}d_{\mu'}-d_{\mu'}H_{\mathrm{QS}})\,|n\rangle\\
&=\langle m|\,\rho_{\mathrm{QS}}\,(t)\,H_{\mathrm{QS}}d_{\mu'}\,|n\rangle-\varepsilon_n\,\langle m|\,\rho_{\mathrm{QS}}\,(t)\,d_{\mu'}\,|n\rangle\,,
\end{aligned} \tag{B.16}$$

若记 $d_{\mu'}\,|n\rangle = |n'\rangle$, 则式 (B.16) 可写为

$$\begin{aligned}
&\langle m|\,\rho_{\mathrm{QS}}\,(t)\,(L_{\mathrm{QS}}d_{\mu'})\,|n\rangle\\
&=\langle m|\,\rho_{\mathrm{QS}}\,(t)\,H_{\mathrm{QS}}\,|n'\rangle-\varepsilon_n\,\langle m|\,\rho_{\mathrm{QS}}\,(t)\,|n'\rangle\\
&=\varepsilon_{n'}\,\langle m|\,\rho_{\mathrm{QS}}\,(t)\,|n'\rangle-\varepsilon_n\,\langle m|\,\rho_{\mathrm{QS}}\,(t)\,|n'\rangle\\
&=(\varepsilon_{n'}-\varepsilon_n)\,\langle m|\,\rho_{\mathrm{QS}}\,(t)\,|n'\rangle\,.
\end{aligned} \tag{B.17}$$

对于 $\langle m|\,\rho_{\mathrm{QS}}\,(t)\,[(L_{\mathrm{QS}})^2\,d_{\mu'}]\,|n\rangle$, 其可以表示为

$$\begin{aligned}
&\langle m|\,\rho_{\mathrm{QS}}\,(t)\,[(L_{\mathrm{QS}})^2\,d_{\mu'}]\,|n\rangle\\
&=\langle m|\,\rho_{\mathrm{QS}}\,(t)\,H_{\mathrm{QS}}\,(H_{\mathrm{QS}}d_{\mu'}-d_{\mu'}H_{\mathrm{QS}})\,|n\rangle\\
&\quad-\langle m|\,\rho_{\mathrm{QS}}\,(t)\,(H_{\mathrm{QS}}d_{\mu'}-d_{\mu'}H_{\mathrm{QS}})\,H_{\mathrm{QS}}\,|n\rangle\\
&=\langle m|\,\rho_{\mathrm{QS}}\,(t)\,H_{\mathrm{QS}}H_{\mathrm{QS}}\,|n'\rangle-\varepsilon_n\,\langle m|\,\rho_{\mathrm{QS}}\,(t)\,H_{\mathrm{QS}}d_{\mu'}\,|n\rangle\\
&\quad-\varepsilon_n\,\langle m|\,\rho_{\mathrm{QS}}\,(t)\,(H_{\mathrm{QS}}d_{\mu'}-d_{\mu'}H_{\mathrm{QS}})\,|n\rangle\\
&=(\varepsilon_{n'})^2\,\langle m|\,\rho_{\mathrm{QS}}\,(t)\,|n'\rangle-\varepsilon_n\,\langle m|\,\rho_{\mathrm{QS}}\,(t)\,H_{\mathrm{QS}}\,|n'\rangle\\
&\quad-\varepsilon_n\,(\varepsilon_{n'}-\varepsilon_n)\,\langle m|\,\rho_{\mathrm{QS}}\,(t)\,|n'\rangle
\end{aligned}$$

$$= (\varepsilon_{n'} - \varepsilon_n)^2 \langle m'| \rho_{\text{QS}}(t) |n\rangle, \tag{B.18}$$

对于 $\langle m| \rho_{\text{QS}}(t) [(L_{\text{QS}})^3 d_{\mu'}] |n\rangle$, 其可以表示为

$$\begin{aligned} &\langle m| \rho_{\text{QS}}(t) [(L_{\text{QS}})^3 d_{\mu'}] |n\rangle \\ =& \langle m| \rho_{\text{QS}}(t) H_{\text{QS}} H_{\text{QS}} (H_{\text{QS}} d_{\mu'} - d_{\mu'} H_{\text{QS}}) |n\rangle \\ &- 2 \langle m| \rho_{\text{QS}}(t) H_{\text{QS}} (H_{\text{QS}} d_{\mu'} - d_{\mu'} H_{\text{QS}}) H_{\text{QS}} |n\rangle \\ &+ \langle m| \rho_{\text{QS}}(t) (H_{\text{QS}} d_{\mu'} - d_{\mu'} H_{\text{QS}}) H_{\text{QS}} H_{\text{QS}} |n\rangle, \end{aligned} \tag{B.19}$$

将上式进一步简化可得

$$\begin{aligned} &\langle m| \rho_{\text{QS}}(t) [(L_{\text{QS}})^3 d_{\mu'}] |n\rangle \\ =& \langle m| \rho_{\text{QS}}(t) H_{\text{QS}} H_{\text{QS}} H_{\text{QS}} |n'\rangle - \varepsilon_n \langle m| \rho_{\text{QS}}(t) H_{\text{QS}} H_{\text{QS}} d_{\mu'} |n\rangle \\ &- 2\varepsilon_n \langle m| \rho_{\text{QS}}(t) H_{\text{QS}} H_{\text{QS}} d_{\mu'} |n\rangle + 2\varepsilon_n \langle m| \rho_{\text{QS}}(t) H_{\text{QS}} d_{\mu'} H_{\text{QS}} |n\rangle \\ &+ (\varepsilon_n)^2 \langle m| \rho_{\text{QS}}(t) (H_{\text{QS}} d_{\mu'} - d_{\mu'} H_{\text{QS}}) |n\rangle \\ =& (\varepsilon_{n'})^3 \langle m| \rho_{\text{QS}}(t) |n'\rangle - \varepsilon_n \langle m| \rho_{\text{QS}}(t) H_{\text{QS}} H_{\text{QS}} |n'\rangle \\ &- 2\varepsilon_n \langle m| \rho_{\text{QS}}(t) H_{\text{QS}} H_{\text{QS}} |n'\rangle + 2 (\varepsilon_n)^2 \langle m| \rho_{\text{QS}}(t) H_{\text{QS}} d_{\mu'} |n\rangle \\ &+ (\varepsilon_n)^2 (\varepsilon_{n'} - \varepsilon_n) \langle m| \rho_{\text{QS}}(t) |n'\rangle \\ =& (\varepsilon_{n'})^3 \langle m| \rho_{\text{QS}}(t) |n'\rangle - (\varepsilon_{n'})^2 \varepsilon_n \langle m| \rho_{\text{QS}}(t) |n'\rangle \\ &- 2 (\varepsilon_{n'})^2 \varepsilon_n \langle m| \rho_{\text{QS}}(t) |n'\rangle + 2\varepsilon_{n'} (\varepsilon_n)^2 \langle m| \rho_{\text{QS}}(t) |n'\rangle \\ &+ (\varepsilon_n)^2 (\varepsilon_{n'} - \varepsilon_n) \langle m| \rho_{\text{QS}}(t) |n'\rangle \\ =& (\varepsilon_{n'} - \varepsilon_n)^3 \langle m| \rho_{\text{QS}}(t) |n'\rangle, \end{aligned} \tag{B.20}$$

同理, 可以证明

$$\langle m| \rho_{\text{QS}}(t) [(L_{\text{QS}})^k d_{\mu'}] |n\rangle = (\varepsilon_{n'} - \varepsilon_n)^k \langle m| \rho_{\text{QS}}(t) |n'\rangle. \tag{B.21}$$

因此, 式 (B.3) 可以写为

$$\langle m| \rho_{\text{QS}}(t) [f_\alpha^{(\pm)}(L_{\text{QS}}) d_{\mu'}] |n\rangle = f_\alpha^{(\pm)}(\varepsilon_{n'} - \varepsilon_n) \langle m| \rho_{\text{QS}}(t) |n'\rangle, \tag{B.22}$$

其中

$$d_{\mu'} |n\rangle = |n'\rangle. \tag{B.23}$$

同理, 式 (B.4) 可以写为

$$\langle m| \rho_{\text{QS}}(t) [f_\alpha^{(\pm)}(L_{\text{QS}}) d_{\mu'}^\dagger] |n\rangle = f_\alpha^{(\pm)}(\varepsilon_{n''} - \varepsilon_n) \langle m| \rho_{\text{QS}}(t) |n''\rangle. \tag{B.24}$$

其中

$$d_{\mu'}^\dagger |n\rangle = |n''\rangle. \tag{B.25}$$

# 附录 C　超算符方程 (2.113) 的形式解

在本附录中给出式 (2.113)

$$\frac{\partial}{\partial t}Q\rho_{\mathrm{I}}(t)=QL_{\mathrm{I}}(t)P\rho_{\mathrm{I}}(t)+QL_{\mathrm{I}}(t)Q\rho_{\mathrm{I}}(t), \tag{C.1}$$

的形式解. 对式 (C.1) 两边分别求关于时间 $t$ 的积分可得

$$Q\rho_{\mathrm{I}}(t)=Q\rho_{\mathrm{I}}(t_0)+\int_{t_0}^{t}\mathrm{d}t_1QL_{\mathrm{I}}(t_1)P\rho_{\mathrm{I}}(t_1)+\int_{t_0}^{t}\mathrm{d}t_1QL_{\mathrm{I}}(t_1)Q\rho_{\mathrm{I}}(t_1), \tag{C.2}$$

将式 (C.2) 中 $t_1\to t_2$ 和 $t\to t_1$ 可得

$$Q\rho_{\mathrm{I}}(t_1)=Q\rho_{\mathrm{I}}(t_0)+\int_{t_0}^{t_1}\mathrm{d}t_2QL_{\mathrm{I}}(t_2)P\rho_{\mathrm{I}}(t_2)+\int_{t_0}^{t_1}\mathrm{d}t_2QL_{\mathrm{I}}(t_2)Q\rho_{\mathrm{I}}(t_2), \tag{C.3}$$

将式 (C.3) 代入式 (C.2) 可得

$$\begin{aligned}
&Q\rho_{\mathrm{I}}(t)\\
&=Q\rho_{\mathrm{I}}(t_0)+\int_{t_0}^{t}\mathrm{d}t_1QL_{\mathrm{I}}(t_1)Q\rho_{\mathrm{I}}(t_0)+\int_{t_0}^{t}\mathrm{d}t_1QL_{\mathrm{I}}(t_1)P\rho_{\mathrm{I}}(t_1)\\
&\quad+\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2QL_{\mathrm{I}}(t_1)QL_{\mathrm{I}}(t_2)P\rho_{\mathrm{I}}(t_2)\\
&\quad+\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2QL_{\mathrm{I}}(t_1)QL_{\mathrm{I}}(t_2)Q\rho_{\mathrm{I}}(t_2).
\end{aligned} \tag{C.4}$$

将式 (C.3) 中 $t_2\to t_3$ 和 $t_1\to t_2$ 可得

$$Q\rho_{\mathrm{I}}(t_2)=Q\rho_{\mathrm{I}}(t_0)+\int_{t_0}^{t_2}\mathrm{d}t_3QL_{\mathrm{I}}(t_3)P\rho_{\mathrm{I}}(t_3)+\int_{t_0}^{t_2}\mathrm{d}t_3QL_{\mathrm{I}}(t_3)Q\rho_{\mathrm{I}}(t_3), \tag{C.5}$$

将式 (C.5) 代入式 (C.4) 可得

$$\begin{aligned}
&Q\rho_{\mathrm{I}}(t)\\
&=\left[1+\int_{t_0}^{t}\mathrm{d}t_1QL_{\mathrm{I}}(t_1)+\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2QL_{\mathrm{I}}(t_1)QL_{\mathrm{I}}(t_2)\right]Q\rho_{\mathrm{I}}(t_0)\\
&\quad+\int_{t_0}^{t}\mathrm{d}t_1QL_{\mathrm{I}}(t_1)P\rho_{\mathrm{I}}(t_1)\\
&\quad+\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2QL_{\mathrm{I}}(t_1)QL_{\mathrm{I}}(t_2)P\rho_{\mathrm{I}}(t_2)\\
&\quad+\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3QL_{\mathrm{I}}(t_1)QL_{\mathrm{I}}(t_2)QL_{\mathrm{I}}(t_3)P\rho_{\mathrm{I}}(t_3)
\end{aligned}$$

$$+\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 QL_{\mathrm{I}}(t_1)QL_{\mathrm{I}}(t_2)QL_{\mathrm{I}}(t_3)Q\rho_{\mathrm{I}}(t_3). \tag{C.6}$$

继续将 $Q\rho_{\mathrm{I}}(t_3)$ 代入式 (C.6), 并重复上面的过程, 最后可得 [2,3]

$$Q\rho_{\mathrm{I}}(t)=G_{\leftarrow}(t,t_0)Q\rho_{\mathrm{I}}(t_0)+\int_{t_0}^{t}\mathrm{d}sG_{\leftarrow}(t,s)QL_{\mathrm{I}}(s)P\rho_{\mathrm{I}}(s), \tag{C.7}$$

$$G_{\leftarrow}(t,s)\equiv T_{\leftarrow}\exp\left[\int_{s}^{t}\mathrm{d}s'QL_{\mathrm{I}}(s')\right]. \tag{C.8}$$

其中, $T_{\leftarrow}$ 为时序算符, 即它将超算符乘积中的时间变量从右到左依次增加.

# 附录 D　几个超算符的展开和计算

在本附录中, 首先计算超算符 $\sum_2(t)$ 和 $\sum_3(t)$ 的表达式. 根据时序算符 $T_{\leftarrow}$ 和反时序算符 $T_{\rightarrow}$ 的性质可知

$$\begin{aligned}
&\frac{1}{2!}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t}\mathrm{d}t_2T_{\leftarrow}QL(t_1)QL(t_2)\\
=&\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t}\mathrm{d}t_2\Theta(t_1-t_2)QL(t_1)QL(t_2)\\
&+\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t}\mathrm{d}t_2\Theta(t_2-t_1)QL(t_2)QL(t_1)\\
=&\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t}\mathrm{d}t_2\Theta(t_1-t_2)QL(t_1)QL(t_2)(t_1>t_2>t_0)\\
&+\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t}\mathrm{d}t_2\Theta(t_2-t_1)QL(t_2)QL(t_1)(t_2>t_1>t_0)\\
=&\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2QL(t_1)QL(t_2)+\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_1QL(t_2)QL(t_1)\\
=&\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2QL(t_1)QL(t_2)\\
&+\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2QL(t_1)QL(t_2)(t_1\to t_2,t_2\to t_1)\\
=&\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2QL(t_1)QL(t_2),
\end{aligned} \tag{D.1}$$

$$
\begin{aligned}
&\frac{(-1)^2}{2!}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t}\mathrm{d}t_2 T_{\rightarrow}L(t_1)L(t_2)\\
&=\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t}\mathrm{d}t_2\left[\Theta(t_2-t_1)L(t_1)L(t_2)+\Theta(t_1-t_2)L(t_2)L(t_1)\right]\\
&=\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t}\mathrm{d}t_2\Theta(t_2-t_1)L(t_1)L(t_2)(t_2>t_1>t_0)\\
&\quad+\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t}\mathrm{d}t_2\Theta(t_1-t_2)L(t_2)L(t_1)(t_1>t_2>t_0)\\
&=\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_1 L(t_1)L(t_2)+\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2 L(t_2)L(t_1)\\
&=\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2 L(t_2)L(t_1)(t_1\rightarrow t_2,t_2\rightarrow t_1)\ +\frac{1}{2}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2 L(t_2)L(t_1)\\
&=\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2 L(t_2)L(t_1),
\end{aligned}
\tag{D.2}
$$

其中, 在上面的推导过程中, 利用了阶跃函数 $\Theta(x)$ 的性质, 其定义为

$$
\Theta(x)=\begin{cases}1, & x>0\\ 0, & x<0\\ 1/2, & x=0\end{cases}.
\tag{D.3}
$$

因此, 开放量子系统向前和向后的传播子可以表示为

$$
\begin{aligned}
G_{\leftarrow}(t,t_1)&\equiv T_{\leftarrow}\exp\left[\int_{t_1}^{t}\mathrm{d}t_2 QL_{\mathrm{I}}(t_2)\right]\\
&=1+\frac{1}{1!}\int_{t_1}^{t}\mathrm{d}t_2 QL_{\mathrm{I}}(t_2)+\frac{1}{2!}\int_{t_1}^{t}\mathrm{d}t_2\int_{t_1}^{t}\mathrm{d}t_3 T_{\leftarrow}QL_{\mathrm{I}}(t_2)QL_{\mathrm{I}}(t_3)+\cdots\\
&=1+\int_{t_1}^{t}\mathrm{d}t_2 QL_{\mathrm{I}}(t_2)+\int_{t_1}^{t}\mathrm{d}t_2\int_{t_1}^{t_2}\mathrm{d}t_3 QL_{\mathrm{I}}(t_2)QL_{\mathrm{I}}(t_3)+\cdots,
\end{aligned}
\tag{D.4}
$$

$$
\begin{aligned}
G_{\rightarrow}(t,t_1)&\equiv T_{\rightarrow}\exp\left[-\int_{t_1}^{t}\mathrm{d}t_2 L_{\mathrm{I}}(t_2)\right]\\
&=1-\int_{t_1}^{t}\mathrm{d}t_2 L_{\mathrm{I}}(t_2)+\frac{1}{2}\int_{t_1}^{t}\mathrm{d}t_2\int_{t_1}^{t}\mathrm{d}t_3 T_{\rightarrow}L_{\mathrm{I}}(t_2)L_{\mathrm{I}}(t_3)+\cdots\\
&=1-\int_{t_1}^{t}\mathrm{d}t_2 L_{\mathrm{I}}(t_2)+\int_{t_1}^{t}\mathrm{d}t_2\int_{t_1}^{t_2}\mathrm{d}t_3 L_{\mathrm{I}}(t_3)L_{\mathrm{I}}(t_2)+\cdots,
\end{aligned}
\tag{D.5}
$$

由超算符 $\sum(t)$ 的定义

$$
\sum(t)=\int_{t_0}^{t}\mathrm{d}t_1 G_{\leftarrow}(t,t_1)QL_{\mathrm{I}}(t_1)PG_{\rightarrow}(t,t_1),
\tag{D.6}
$$

以及式 (D.4) 和 (D.5) 可知, 其二阶项可表示为

$$
\begin{aligned}
\sum_2(t) &\overset{t_1\leq t_2}{=} \int_{t_0}^{t}\mathrm{d}t_1\int_{t_1}^{t}\mathrm{d}t_2 QL_{\mathrm{I}}(t_2)QL_{\mathrm{I}}(t_1)P-\int_{t_0}^{t}\mathrm{d}t_1\int_{t_1}^{t}\mathrm{d}t_2 QL_{\mathrm{I}}(t_1)PL_{\mathrm{I}}(t_2)\\
&\underset{t_1>t_2}{\overset{t_1\leftrightarrow t_2}{=}} \int_{t_0}^{t}\mathrm{d}t_2\int_{t_2}^{t}\mathrm{d}t_1 QL_{\mathrm{I}}(t_1)QL_{\mathrm{I}}(t_2)P-\int_{t_0}^{t}\mathrm{d}t_2\int_{t_2}^{t}\mathrm{d}t_1 QL_{\mathrm{I}}(t_2)PL_{\mathrm{I}}(t_1)\\
&=\left(\int_{t_0}^{t_1}\mathrm{d}t_2+\overbrace{\int_{t_1}^{t}\mathrm{d}t_2}^{=0}\right)\left(\overbrace{\int_{t_0}^{t_2}\mathrm{d}t_1}^{=0}+\int_{t_2}^{t}\mathrm{d}t_1\right)\\
&\quad\times\left[QL_{\mathrm{I}}(t_1)QL_{\mathrm{I}}(t_2)P-QL_{\mathrm{I}}(t_2)PL_{\mathrm{I}}(t_1)\right]\\
&=\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\left[QL_{\mathrm{I}}(t_1)QL_{\mathrm{I}}(t_2)P-QL_{\mathrm{I}}(t_2)PL_{\mathrm{I}}(t_1)\right]\\
&=\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\left[QL_{\mathrm{I}}(t_1)L_{\mathrm{I}}(t_2)P-L_{\mathrm{I}}(t_2)PL_{\mathrm{I}}(t_1)\right],
\end{aligned}\tag{D.7}
$$

其中, 上式推导中利用了超算符的性质 $PL_{\mathrm{I}}(t)P=0$.

同样, 超算符 $\sum(t)$ 的三阶项 $\sum\limits_3(t)$ 可表示为

$$
\begin{aligned}
\sum_3(t)=&-\overbrace{\int_{t_0}^{t}\mathrm{d}t_1\int_{t_1}^{t}\mathrm{d}t_2\int_{t_1}^{t}\mathrm{d}t_3 QL_{\mathrm{I}}(t_2)QL_{\mathrm{I}}(t_1)PL_{\mathrm{I}}(t_3)}^{t>t_2>t_3>t_1>t_0}\\
&-\overbrace{\int_{t_0}^{t}\mathrm{d}t_1\int_{t_1}^{t}\mathrm{d}t_2\int_{t_1}^{t}\mathrm{d}t_3 QL_{\mathrm{I}}(t_2)QL_{\mathrm{I}}(t_1)PL_{\mathrm{I}}(t_3)}^{t>t_3>t_2>t_1>t_0}\\
&+\overbrace{\int_{t_0}^{t}\mathrm{d}t_1\int_{t_1}^{t}\mathrm{d}t_2\int_{t_1}^{t_2}\mathrm{d}t_3 QL_{\mathrm{I}}(t_2)QL_{\mathrm{I}}(t_3)QL_{\mathrm{I}}(t_1)P}^{t>t_2>t_3>t_1>t_0}\\
&+\overbrace{\int_{t_0}^{t}\mathrm{d}t_1\int_{t_1}^{t}\mathrm{d}t_2\int_{t_1}^{t_2}\mathrm{d}t_3 QL_{\mathrm{I}}(t_1)PL_{\mathrm{I}}(t_3)L_{\mathrm{I}}(t_2)}^{t>t_2>t_3>t_1>t_0},
\end{aligned}\tag{D.8}
$$

其中, 式 (D.8) 右边的第一项到第四项可分别表示为

$$
\left.\sum_3(t)\right|_{01}=-\overbrace{\int_{t_0}^{t}\mathrm{d}t_1\int_{t_1}^{t}\mathrm{d}t_2\int_{t_1}^{t}\mathrm{d}t_3 QL_{\mathrm{I}}(t_2)QL_{\mathrm{I}}(t_1)PL_{\mathrm{I}}(t_3)}^{t>t_2>t_3>t_1>t_0}
$$

$$
\begin{aligned}
&\overset{t_2\leftrightarrow t_1}{=} -\overbrace{\int_{t_0}^{t}\mathrm{d}t_2\int_{t_2}^{t}\mathrm{d}t_1\int_{t_2}^{t}\mathrm{d}t_3 QL_{\mathrm{I}}\left(t_1\right)QL_{\mathrm{I}}\left(t_2\right)PL_{\mathrm{I}}\left(t_3\right)}^{t>t_1>t_3>t_2>t_0}\\
&\overset{t_2\leftrightarrow t_3}{=} -\overbrace{\int_{t_3}^{t}\mathrm{d}t_1\int_{t_3}^{t}\mathrm{d}t_2\int_{t_0}^{t}\mathrm{d}t_3 QL_{\mathrm{I}}\left(t_1\right)QL_{\mathrm{I}}\left(t_3\right)PL_{\mathrm{I}}\left(t_2\right)}^{t>t_1>t_2>t_3>t_0}\\
&= -\left(\overbrace{\int_{t_0}^{t_3}\mathrm{d}t_1}^{=0}+\int_{t_3}^{t}\mathrm{d}t_1\right)\left(\overbrace{\int_{t_0}^{t_3}\mathrm{d}t_2}^{=0}+\int_{t_3}^{t_1}\mathrm{d}t_2+\overbrace{\int_{t_1}^{t}\mathrm{d}t_2}^{=0}\right)\left(\int_{t_0}^{t_2}\mathrm{d}t_3+\overbrace{\int_{t_2}^{t}\mathrm{d}t_3}^{=0}\right)\\
&\quad\times QL_{\mathrm{I}}\left(t_1\right)QL_{\mathrm{I}}\left(t_3\right)PL_{\mathrm{I}}\left(t_2\right)\\
&= -\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 QL_{\mathrm{I}}\left(t_1\right)QL_{\mathrm{I}}\left(t_3\right)PL_{\mathrm{I}}\left(t_2\right),
\end{aligned}
\tag{D.9}
$$

$$
\begin{aligned}
\left.\sum_3(t)\right|_{02} &= -\overbrace{\int_{t_0}^{t}\mathrm{d}t_1\int_{t_1}^{t}\mathrm{d}t_2\int_{t_1}^{t}\mathrm{d}t_3 QL_{\mathrm{I}}\left(t_2\right)QL_{\mathrm{I}}\left(t_1\right)PL_{\mathrm{I}}\left(t_3\right)}^{t>t_3>t_2>t_1>t_0}\\
&\overset{t_3\leftrightarrow t_1}{=} -\overbrace{\int_{t_3}^{t}\mathrm{d}t_1\int_{t_3}^{t}\mathrm{d}t_2\int_{t_0}^{t}\mathrm{d}t_3 QL_{\mathrm{I}}\left(t_2\right)QL_{\mathrm{I}}\left(t_3\right)PL_{\mathrm{I}}\left(t_1\right)}^{t>t_1>t_2>t_3>t_0}\\
&= -\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 QL_{\mathrm{I}}\left(t_2\right)QL_{\mathrm{I}}\left(t_3\right)PL_{\mathrm{I}}\left(t_1\right),
\end{aligned}
\tag{D.10}
$$

$$
\begin{aligned}
\left.\sum_3(t)\right|_{03} &= \overbrace{\int_{t_0}^{t}\mathrm{d}t_1\int_{t_1}^{t}\mathrm{d}t_2\int_{t_1}^{t_2}\mathrm{d}t_3 QL_{\mathrm{I}}\left(t_2\right)QL_{\mathrm{I}}\left(t_3\right)QL_{\mathrm{I}}\left(t_1\right)P}^{t>t_2>t_3>t_1>t_0}\\
&\overset{t_1\leftrightarrow t_2}{=} \overbrace{\int_{t_0}^{t}\mathrm{d}t_2\int_{t_2}^{t}\mathrm{d}t_1\int_{t_2}^{t_1}\mathrm{d}t_3 QL_{\mathrm{I}}\left(t_1\right)QL_{\mathrm{I}}\left(t_3\right)QL_{\mathrm{I}}\left(t_2\right)P}^{t>t_1>t_3>t_2>t_0}\\
&\overset{t_2\leftrightarrow t_3}{=} \overbrace{\int_{t_3}^{t}\mathrm{d}t_1\int_{t_3}^{t_1}\mathrm{d}t_2\int_{t_0}^{t}\mathrm{d}t_3 QL_{\mathrm{I}}\left(t_1\right)QL_{\mathrm{I}}\left(t_2\right)QL_{\mathrm{I}}\left(t_3\right)P}^{t>t_1>t_2>t_3>t_0}\\
&= \int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 QL_{\mathrm{I}}\left(t_1\right)QL_{\mathrm{I}}\left(t_2\right)QL_{\mathrm{I}}\left(t_3\right)P,
\end{aligned}
\tag{D.11}
$$

$$
\left.\sum_3(t)\right|_{04} = \overbrace{\int_{t_0}^{t}\mathrm{d}t_1\int_{t_1}^{t}\mathrm{d}t_2\int_{t_1}^{t_2}\mathrm{d}t_3 QL_{\mathrm{I}}\left(t_1\right)PL_{\mathrm{I}}\left(t_3\right)L_{\mathrm{I}}\left(t_2\right)}^{t>t_2>t_3>t_1>t_0}
$$

$$
\begin{aligned}
&\overset{t_1\leftrightarrow t_2}{=} \overbrace{\int_{t_0}^{t}\mathrm{d}t_2\int_{t_2}^{t}\mathrm{d}t_1\int_{t_2}^{t_1}\mathrm{d}t_3 QL_{\mathrm{I}}\left(t_2\right)PL_{\mathrm{I}}\left(t_3\right)L_{\mathrm{I}}\left(t_1\right)}^{t>t_1>t_3>t_2>t_0}\\
&\overset{t_2\leftrightarrow t_3}{=} \overbrace{\int_{t_3}^{t}\mathrm{d}t_1\int_{t_3}^{t_1}\mathrm{d}t_2\int_{t_0}^{t}\mathrm{d}t_3 QL_{\mathrm{I}}\left(t_3\right)PL_{\mathrm{I}}\left(t_2\right)L_{\mathrm{I}}\left(t_1\right)}^{t>t_1>t_2>t_3>t_0}\\
&=\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 QL_{\mathrm{I}}\left(t_3\right)PL_{\mathrm{I}}\left(t_2\right)L_{\mathrm{I}}\left(t_1\right).
\end{aligned}\tag{D.12}
$$

因而, 超算符 $\sum(t)$ 的三阶项 $\sum\limits_{3}(t)$ 最后可表示为

$$
\begin{aligned}
\sum_{3}(t)=&\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\left[-QL_{\mathrm{I}}\left(t_1\right)L_{\mathrm{I}}\left(t_3\right)PL_{\mathrm{I}}\left(t_2\right)-QL_{\mathrm{I}}\left(t_2\right)L_{\mathrm{I}}\left(t_3\right)PL_{\mathrm{I}}\left(t_1\right)\right.\\
&\left.+QL_{\mathrm{I}}\left(t_1\right)QL_{\mathrm{I}}\left(t_2\right)L_{\mathrm{I}}\left(t_3\right)P+QL_{\mathrm{I}}\left(t_3\right)PL_{\mathrm{I}}\left(t_2\right)L_{\mathrm{I}}\left(t_1\right)\right].
\end{aligned}\tag{D.13}
$$

利用超算符的性质 $PL_{\mathrm{I}}(t)P=0$ 和 $PQ=0$, 超算符 $\sum\limits_{2}(t)\sum\limits_{1}(t)$ 可表示为

$$
\begin{aligned}
&\sum_{2}(t)\sum_{1}(t)\\
&=\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t}\mathrm{d}t_3\left[QL_{\mathrm{I}}\left(t_1\right)L_{\mathrm{I}}\left(t_2\right)P-L_{\mathrm{I}}\left(t_2\right)PL_{\mathrm{I}}\left(t_1\right)\right]QL_{\mathrm{I}}\left(t_3\right)P\\
&=-\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t}\mathrm{d}t_3 L_{\mathrm{I}}\left(t_2\right)PL_{\mathrm{I}}\left(t_1\right)L_{\mathrm{I}}\left(t_3\right)P,
\end{aligned}\tag{D.14}
$$

考虑到时间变量的大小, 可将式 (D.14) 表示为如下形式:

$$
\begin{aligned}
&\sum_{2}(t)\sum_{1}(t)\\
&=-\overbrace{\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t}\mathrm{d}t_3 L_{\mathrm{I}}\left(t_2\right)PL_{\mathrm{I}}\left(t_1\right)L_{\mathrm{I}}\left(t_3\right)P}^{t>t_3>t_1>t_2>t_0}\\
&\quad-\overbrace{\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t}\mathrm{d}t_3 L_{\mathrm{I}}\left(t_2\right)PL_{\mathrm{I}}\left(t_1\right)L_{\mathrm{I}}\left(t_3\right)P}^{t>t_1>t_3>t_2>t_0}\\
&\quad-\overbrace{\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t}\mathrm{d}t_3 L_{\mathrm{I}}\left(t_2\right)PL_{\mathrm{I}}\left(t_1\right)L_{\mathrm{I}}\left(t_3\right)P}^{t>t_1>t_2>t_3>t_0},
\end{aligned}\tag{D.15}
$$

其中, 式 (D.15) 右边的第一项到第三项可分别表示为

$$
\begin{aligned}
&\sum_2(t)\sum_1(t)\bigg|_{01}\\
&=-\overbrace{\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t}\mathrm{d}t_3 L_{\mathrm{I}}(t_2)PL_{\mathrm{I}}(t_1)L_{\mathrm{I}}(t_3)P}^{t>t_3>t_1>t_2>t_0}\\
&\overset{t_3\leftrightarrow t_1}{=}-\overbrace{\int_{t_0}^{t}\mathrm{d}t_3\int_{t_0}^{t_3}\mathrm{d}t_2\int_{t_0}^{t}\mathrm{d}t_1 L_{\mathrm{I}}(t_2)PL_{\mathrm{I}}(t_3)L_{\mathrm{I}}(t_1)P}^{t>t_1>t_3>t_2>t_0}\\
&\overset{t_3\leftrightarrow t_2}{=}-\overbrace{\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 L_{\mathrm{I}}(t_3)PL_{\mathrm{I}}(t_2)L_{\mathrm{I}}(t_1)P}^{t>t_1>t_2>t_3>t_0}\\
&=-\int_{t_0}^{t}\mathrm{d}t_1\left(\int_{t_0}^{t_1}\mathrm{d}t_2+\overbrace{\int_{t_1}^{t}\mathrm{d}t_2}^{=0}\right)\int_{t_0}^{t_2}\mathrm{d}t_3 L_{\mathrm{I}}(t_3)PL_{\mathrm{I}}(t_2)L_{\mathrm{I}}(t_1)P\\
&=-\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 L_{\mathrm{I}}(t_3)PL_{\mathrm{I}}(t_2)L_{\mathrm{I}}(t_1)P,
\end{aligned}
\tag{D.16}
$$

$$
\begin{aligned}
&\sum_2(t)\sum_1(t)\bigg|_{02}\\
&=-\overbrace{\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t}\mathrm{d}t_3 L_{\mathrm{I}}(t_2)PL_{\mathrm{I}}(t_1)L_{\mathrm{I}}(t_3)P}^{t>t_1>t_3>t_2>t_0}\\
&\overset{t_3\leftrightarrow t_2}{=}-\overbrace{\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t}\mathrm{d}t_2\int_{t_0}^{t_1}\mathrm{d}t_3 L_{\mathrm{I}}(t_3)PL_{\mathrm{I}}(t_1)L_{\mathrm{I}}(t_2)P}^{t>t_1>t_2>t_3>t_0}\\
&=-\int_{t_0}^{t}\mathrm{d}t_1\left(\int_{t_0}^{t_1}\mathrm{d}t_2+\overbrace{\int_{t_1}^{t}\mathrm{d}t_2}^{=0}\right)\left(\int_{t_0}^{t_2}\mathrm{d}t_3+\overbrace{\int_{t_2}^{t_1}\mathrm{d}t_3}^{=0}\right)L_{\mathrm{I}}(t_3)PL_{\mathrm{I}}(t_1)L_{\mathrm{I}}(t_2)P\\
&=-\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 L_{\mathrm{I}}(t_3)PL_{\mathrm{I}}(t_1)L_{\mathrm{I}}(t_2)P,
\end{aligned}
\tag{D.17}
$$

$$\begin{aligned}
&\sum_2(t)\sum_1(t)\bigg|_{03}\\
&=-\overbrace{\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t}\mathrm{d}t_3 L_{\mathrm{I}}(t_2)PL_{\mathrm{I}}(t_1)L_{\mathrm{I}}(t_3)P}^{t>t_1>t_2>t_3>t_0}\\
&=-\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\left(\int_{t_0}^{t_2}\mathrm{d}t_3+\overbrace{\int_{t_2}^{t}\mathrm{d}t_3}^{=0}\right)L_{\mathrm{I}}(t_2)PL_{\mathrm{I}}(t_1)L_{\mathrm{I}}(t_3)P\\
&=-\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 L_{\mathrm{I}}(t_2)PL_{\mathrm{I}}(t_1)L_{\mathrm{I}}(t_3)P,
\end{aligned}\tag{D.18}$$

因而, 超算符 $\sum\limits_2(t)\sum\limits_1(t)$ 最后可表示为

$$\begin{aligned}
\sum_2(t)\sum_1(t)=&-\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\left[L_{\mathrm{I}}(t_3)PL_{\mathrm{I}}(t_2)L_{\mathrm{I}}(t_1)P\right.\\
&\left.+L_{\mathrm{I}}(t_3)PL_{\mathrm{I}}(t_1)L_{\mathrm{I}}(t_2)P+L_{\mathrm{I}}(t_2)PL_{\mathrm{I}}(t_1)L_{\mathrm{I}}(t_3)P\right].
\end{aligned}\tag{D.19}$$

根据式 (D.19), 超算符 $PL_{\mathrm{I}}(t)\sum\limits_2(t)\sum\limits_1(t)P$ 可表示为

$$\begin{aligned}
&PL_{\mathrm{I}}(t)\sum_2(t)\sum_1(t)P\\
&=-\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 PL_{\mathrm{I}}(t)\left[L_{\mathrm{I}}(t_3)PL_{\mathrm{I}}(t_2)L_{\mathrm{I}}(t_1)P\right.\\
&\quad\left.+L_{\mathrm{I}}(t_3)PL_{\mathrm{I}}(t_1)L_{\mathrm{I}}(t_2)P+L_{\mathrm{I}}(t_2)PL_{\mathrm{I}}(t_1)L_{\mathrm{I}}(t_3)P\right]P\\
&=-\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 PL_{\mathrm{I}}(t)\left[L_{\mathrm{I}}(t_2)PL_{\mathrm{I}}(t_1)L_{\mathrm{I}}(t_3)P\right.\\
&\quad\left.+L_{\mathrm{I}}(t_3)PL_{\mathrm{I}}(t_2)L_{\mathrm{I}}(t_1)P+L_{\mathrm{I}}(t_3)PL_{\mathrm{I}}(t_1)L_{\mathrm{I}}(t_2)P\right],
\end{aligned}\tag{D.20}$$

同理, 超算符 $PL_{\mathrm{I}}(t)\sum\limits_3(t)P$ 可表示为

$$\begin{aligned}
&PL_{\mathrm{I}}(t)\sum_3(t)P\\
&=-\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 PL_{\mathrm{I}}(t)QL_{\mathrm{I}}(t_1)QL_{\mathrm{I}}(t_3)PL_{\mathrm{I}}(t_2)P\\
&\quad-\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 PL_{\mathrm{I}}(t)QL_{\mathrm{I}}(t_2)QL_{\mathrm{I}}(t_3)PL_{\mathrm{I}}(t_1)P\\
&\quad+\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 PL_{\mathrm{I}}(t)QL_{\mathrm{I}}(t_1)QL_{\mathrm{I}}(t_2)QL_{\mathrm{I}}(t_3)PP
\end{aligned}$$

$$
\begin{aligned}
&+\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 PL_{\mathrm{I}}(t)\,QL_{\mathrm{I}}(t_3)\,PL_{\mathrm{I}}(t_2)\,L_{\mathrm{I}}(t_1)\,P\\
=&\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 PL_{\mathrm{I}}(t)\,L_{\mathrm{I}}(t_1)\,QL_{\mathrm{I}}(t_2)\,L_{\mathrm{I}}(t_3)\,P\\
&+\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3 PL_{\mathrm{I}}(t)\,L_{\mathrm{I}}(t_3)\,PL_{\mathrm{I}}(t_2)\,L_{\mathrm{I}}(t_1)\,P. \qquad \text{(D.21)}
\end{aligned}
$$

# 附录 E　与非马尔可夫效应相关的一个主值积分

在本附录中, 计算与式 (2.170) 右边第二项相关的主值积分

$$
\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha(\omega)\,f_\alpha(\omega)\cos[(\omega-\Delta)\,t/\hbar]}{\omega-\Delta}\\
=&W^2P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{1}{1+\mathrm{e}^{\frac{\omega-\mu_\alpha}{k_{\mathrm{B}}T}}}\frac{1}{\omega-\Delta}\frac{1}{\omega-\mu_\alpha-\mathrm{i}W}\frac{1}{\omega-\mu_\alpha+\mathrm{i}W}\cos[(\omega-\Delta)\,t/\hbar], \qquad \text{(E.1)}\\
&P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha(\omega)\,f_\alpha(\omega)\sin[(\omega-\Delta)\,t/\hbar]}{\omega-\Delta}\\
=&W^2P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{1}{1+\mathrm{e}^{\frac{\omega-\mu_\alpha}{k_{\mathrm{B}}T}}}\frac{1}{\omega-\Delta}\frac{1}{\omega-\mu_\alpha-\mathrm{i}W}\frac{1}{\omega-\mu_\alpha+\mathrm{i}W}\sin[(\omega-\Delta)\,t/\hbar]. \qquad \text{(E.2)}
\end{aligned}
$$

为方便计算, 令 $\beta=1/k_{\mathrm{B}}T$, 且 $x=\beta(\omega-\mu_\alpha)$, 则式 (E.1) 可以写为

$$
\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha(\omega)\,f_\alpha(\omega)\cos[(\omega-\Delta)\,t/\hbar]}{\omega-\Delta}\\
=&(\beta W)^2P\int_{-\infty}^{\infty}\mathrm{d}x\frac{1}{1+\mathrm{e}^{x}}\frac{1}{x-x_1}\frac{1}{x-x_2}\frac{1}{x-x_3}\cos[(x-x_1)\,t/\hbar], \qquad \text{(E.3)}
\end{aligned}
$$

其中

$$
\begin{cases}
x_1=\beta(\Delta-\mu_\alpha)\\
x_2=\mathrm{i}\beta W\\
x_3=-\mathrm{i}\beta W
\end{cases}. \qquad \text{(E.4)}
$$

下面利用留数定理计算式 (E.3) 的主值积分, 并将其被积函数写为

$$
f(z)=\frac{1}{1+\mathrm{e}^{z}}\frac{1}{z-x_1}\frac{1}{z-x_2}\frac{1}{z-x_3}\cos[(z-x_1)\,t/\hbar], \qquad \text{(E.5)}
$$

其奇点可以表示为

$$
\begin{cases}
z_{0,n}=\mathrm{i}(2n+1)\,\pi, \quad n=0,\pm1,\pm2,\cdots\\
z_1=x_1\\
z_2=x_2\\
z_3=x_3
\end{cases}, \qquad \text{(E.6)}
$$

其中, $z_{0,n}$ 是虚轴上的一阶奇点, $z_1$ 是实轴上的一阶奇点, $z_2$ 是正虚轴上的一阶奇点, $z_3$ 是负虚轴上的一阶奇点. 积分路径如图 A.1 所示. 由留数定理可知

$$\oint f(z)\mathrm{d}z = 2\pi\mathrm{i}\sum_n \mathrm{Res}\left[f\left(z\right), z_{0,n}\right] + 2\pi\mathrm{i}\mathrm{Res}\left[f\left(z\right), z_2\right], \tag{E.7}$$

其中

$$\begin{aligned}
&\mathrm{Res}\left[f\left(z\right), z_{0,n}\right] \\
&= \cos\left[\left(z_{0,n} - x_1\right)t/\hbar\right]\left[-\frac{1}{x_1 - x_2}\frac{1}{x_1 - x_3}\frac{1}{z_{0,n} - x_1} + \frac{1}{x_1 - x_2}\frac{1}{x_1 - x_3}\frac{1}{z_{0,n} - x_3}\right. \\
&\quad \left. + \frac{1}{x_1 - x_2}\frac{1}{x_2 - x_3}\frac{1}{z_{0,n} - x_2} - \frac{1}{x_1 - x_2}\frac{1}{x_2 - x_3}\frac{1}{z_{0,n} - x_3}\right],
\end{aligned} \tag{E.8}$$

$$\mathrm{Res}\left[f\left(z\right), x_2\right] = \frac{1}{1 + \mathrm{e}^{x_2}}\frac{1}{x_2 - x_1}\frac{1}{x_2 - x_3}\cos\left[\left(x_2 - x_1\right)t/\hbar\right], \tag{E.9}$$

将式 (E.8) 和 (E.9) 代入式 (E.7) 可得

$$\begin{aligned}
&\oint f(z)\mathrm{d}z \\
&= \frac{2\pi\mathrm{i}\cos\left[\left(x_2 - x_1\right)t/\hbar\right]}{\left(1 + \mathrm{e}^{x_2}\right)\left(x_2 - x_1\right)\left(x_2 - x_3\right)} \\
&\quad - \sum_n \frac{2\pi\mathrm{i}\cos\left[\left(z_{0,n} - x_1\right)t/\hbar\right]}{\left(x_1 - x_2\right)\left(x_1 - x_3\right)\left(z_{0,n} - x_1\right)} + \sum_n \frac{2\pi\mathrm{i}\cos\left[\left(z_{0,n} - x_1\right)t/\hbar\right]}{\left(x_1 - x_2\right)\left(x_1 - x_3\right)\left(z_{0,n} - x_3\right)} \\
&\quad + \sum_n \frac{2\pi\mathrm{i}\cos\left[\left(z_{0,n} - x_1\right)t/\hbar\right]}{\left(x_1 - x_2\right)\left(x_2 - x_3\right)\left(z_{0,n} - x_2\right)} - \sum_n \frac{2\pi\mathrm{i}\cos\left[\left(z_{0,n} - x_1\right)t/\hbar\right]}{\left(x_1 - x_2\right)\left(x_2 - x_3\right)\left(z_{0,n} - x_3\right)}.
\end{aligned} \tag{E.10}$$

由于当 $|z| \to \infty$ 时, 积分

$$\lim_{|z|\to\infty} zf\left(z\right) = \lim_{|z|\to\infty} z\frac{1}{1 + \mathrm{e}^z}\frac{1}{z - x_1}\frac{1}{z - x_2}\frac{1}{z - x_3}\cos\left[\left(z - x_1\right)t/\hbar\right] = 0, \tag{E.11}$$

因而有

$$\int_{C_R} f\left(z\right)\mathrm{d}z = 0. \tag{E.12}$$

此外, 积分

$$\int_{C_r} f\left(z\right)\mathrm{d}z = -\mathrm{i}\pi\mathrm{Res}\left[f\left(z\right), x_1\right] = -\mathrm{i}\pi\frac{1}{1 + \mathrm{e}^{x_1}}\frac{1}{x_1 - x_2}\frac{1}{x_1 - x_3}. \tag{E.13}$$

当 $R \to \infty$, 且 $r \to 0$ 时, $f\left(z\right)$ 的主值积分可表示为

$$P\int_{-\infty}^{\infty}\mathrm{d}x\frac{1}{1 + \mathrm{e}^x}\frac{1}{x - x_1}\frac{1}{x - x_2}\frac{1}{x - x_3}\cos\left[\left(z - x_1\right)t/\hbar\right]$$

$$
\begin{aligned}
&= \oint f(z)\mathrm{d}z - \int_{C_R} f(z)\,\mathrm{d}z - \int_{C_r} f(z)\,\mathrm{d}z \\
&= 2\pi\mathrm{i}\frac{\cos\left[\left(x_2-x_1\right)t/\hbar\right]}{\left(1+\mathrm{e}^{x_2}\right)\left(x_2-x_1\right)\left(x_2-x_3\right)} + \pi\mathrm{i}\frac{1}{1+\mathrm{e}^{x_1}}\frac{1}{x_1-x_2}\frac{1}{x_1-x_3} \\
&\quad - \sum_{n=0}^{\infty}\frac{2\pi\mathrm{i}\cos\left[\left(z_{0,n}-x_1\right)t/\hbar\right]}{\left(x_1-x_2\right)\left(x_1-x_3\right)\left(z_{0,n}-x_1\right)} + \sum_{n=0}^{\infty}\frac{2\pi\mathrm{i}\cos\left[\left(z_{0,n}-x_1\right)t/\hbar\right]}{\left(x_1-x_2\right)\left(x_1-x_3\right)\left(z_{0,n}-x_3\right)} \\
&\quad + \sum_{n=0}^{\infty}\frac{2\pi\mathrm{i}\cos\left[\left(z_{0,n}-x_1\right)t/\hbar\right]}{\left(x_1-x_2\right)\left(x_2-x_3\right)\left(z_{0,n}-x_2\right)} - \sum_{n=0}^{\infty}\frac{2\pi\mathrm{i}\cos\left[\left(z_{0,n}-x_1\right)t/\hbar\right]}{\left(x_1-x_2\right)\left(x_2-x_3\right)\left(z_{0,n}-x_3\right)},
\end{aligned}
\tag{E.14}
$$

即

$$
\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha\left(\omega\right)f_\alpha\left(\omega\right)\cos\left[\left(z-x_1\right)t/\hbar\right]}{\omega-\Delta} \\
&= 2\pi\mathrm{i}\frac{\cos\left[\left(x_2-x_1\right)t/\hbar\right]}{\left(1+\mathrm{e}^{x_2}\right)\left(x_2-x_1\right)\left(x_2-x_3\right)} + \pi\mathrm{i}\frac{1}{1+\mathrm{e}^{x_1}}\frac{1}{x_1-x_2}\frac{1}{x_1-x_3} \\
&\quad - \sum_{n=0}^{\infty}\frac{2\pi\mathrm{i}\cos\left[\left(z_{0,n}-x_1\right)t/\hbar\right]}{\left(x_1-x_2\right)\left(x_1-x_3\right)\left(z_{0,n}-x_1\right)} + \sum_{n=0}^{\infty}\frac{2\pi\mathrm{i}\cos\left[\left(z_{0,n}-x_1\right)t/\hbar\right]}{\left(x_1-x_2\right)\left(x_1-x_3\right)\left(z_{0,n}-x_3\right)} \\
&\quad + \sum_{n=0}^{\infty}\frac{2\pi\mathrm{i}\cos\left[\left(z_{0,n}-x_1\right)t/\hbar\right]}{\left(x_1-x_2\right)\left(x_2-x_3\right)\left(z_{0,n}-x_2\right)} - \sum_{n=0}^{\infty}\frac{2\pi\mathrm{i}\cos\left[\left(z_{0,n}-x_1\right)t/\hbar\right]}{\left(x_1-x_2\right)\left(x_2-x_3\right)\left(z_{0,n}-x_3\right)},
\end{aligned}
\tag{E.15}
$$

同理, 可得

$$
\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha\left(\omega\right)f_\alpha\left(\omega\right)\sin\left[\left(z-x_1\right)t/\hbar\right]}{\omega-\Delta} \\
&= 2\pi\mathrm{i}\frac{1}{1+\mathrm{e}^{x_2}}\frac{1}{x_2-x_1}\frac{1}{x_2-x_3}\sin\left[\left(x_2-x_1\right)t/\hbar\right] \\
&\quad - \sum_{n=0}^{\infty}\frac{2\pi\mathrm{i}\sin\left[\left(z_{0,n}-x_1\right)t/\hbar\right]}{\left(x_1-x_2\right)\left(x_1-x_3\right)\left(z_{0,n}-x_1\right)} + \sum_{n=0}^{\infty}\frac{2\pi\mathrm{i}\sin\left[\left(z_{0,n}-x_1\right)t/\hbar\right]}{\left(x_1-x_2\right)\left(x_1-x_3\right)\left(z_{0,n}-x_3\right)} \\
&\quad + \sum_{n=0}^{\infty}\frac{2\pi\mathrm{i}\sin\left[\left(z_{0,n}-x_1\right)t/\hbar\right]}{\left(x_1-x_2\right)\left(x_2-x_3\right)\left(z_{0,n}-x_2\right)} - \sum_{n=0}^{\infty}\frac{2\pi\mathrm{i}\sin\left[\left(z_{0,n}-x_1\right)t/\hbar\right]}{\left(x_1-x_2\right)\left(x_2-x_3\right)\left(z_{0,n}-x_3\right)},
\end{aligned}
\tag{E.16}
$$

上式中的相关参数见式 (E.6).

# 附录 F　电流前四阶累积矩的推导

在本附录中, 基于瑞利–薛定谔微扰理论给出开放量子系统电流前四阶累积矩的具体计算细节 [4]. 设矩阵 $L\left(\chi\right)$ 的本征值和相应本征态分别记为 $\lambda_0\left(\chi\right)$ 和

$|0(\chi)\rangle\rangle$, 则有

$$L(\chi)|0(\chi)\rangle\rangle = \lambda_0(\chi)|0(\chi)\rangle\rangle, \tag{F.1}$$

其中, $\lambda_0(\chi = 0) = 0$. 此外, 令

$$L(\chi) = L_0 + \Delta L(\chi) = L_0 + L_1(\mathrm{i}\chi) + \frac{L_2}{2}(\mathrm{i}\chi)^2 + \frac{L_3}{6}(\mathrm{i}\chi)^3 + \frac{L_4}{24}(\mathrm{i}\chi)^4 + \cdots, \tag{F.2}$$

$$\lambda_0(\chi) = C_1(\mathrm{i}\chi) + \frac{C_2}{2}(\mathrm{i}\chi)^2 + \frac{C_3}{6}(\mathrm{i}\chi)^3 + \frac{C_4}{24}(\mathrm{i}\chi)^4 + \cdots \tag{F.3}$$

由于 $\langle\langle\tilde{0}|L_0 = 0$, 将式 (F.1) 两边左乘以 $\langle\langle\tilde{0}|$ 可得

$$\langle\langle\tilde{0}|[L_0 + \Delta L(\chi)]|0(\chi)\rangle\rangle = \langle\langle\tilde{0}|\Delta L(\chi)|0(\chi)\rangle\rangle = \lambda_0(\chi)\langle\langle\tilde{0}||0(\chi)\rangle\rangle, \tag{F.4}$$

若选择一个非标准的归一化条件

$$\langle\langle\tilde{0}||0(\chi)\rangle\rangle = \langle\langle\tilde{0}||0\rangle\rangle = 1, \tag{F.5}$$

其中 $L_0|0\rangle\rangle = 0$, 即 $\rho^{\text{steady state}} \leftrightarrow |0\rangle\rangle$, 因而 $\lambda_0(\chi)$ 可以表示为

$$\lambda_0(\chi) = \langle\langle\tilde{0}|\Delta L(\chi)|0(\chi)\rangle\rangle. \tag{F.6}$$

若定义超算符 $\tilde{P} = \tilde{P}^2 = |0\rangle\rangle\langle\langle\tilde{0}|$ 和其相应的互补算符 $\tilde{Q} = \tilde{Q}^2 = 1 - |0\rangle\rangle\langle\langle\tilde{0}|$, 则本征态 $|0(\chi)\rangle\rangle$ 可以表示为

$$|0(\chi)\rangle\rangle = |0\rangle\rangle + \tilde{Q}|0(\chi)\rangle\rangle. \tag{F.7}$$

将式 (F.1) 重新表示为

$$L_0|0(\chi)\rangle\rangle = [\lambda_0(\chi) - \Delta L(\chi)]|0(\chi)\rangle\rangle, \tag{F.8}$$

考虑到 $\tilde{Q}L_0\tilde{Q} = \left[1 - |0\rangle\rangle\langle\langle\tilde{0}|\right] L_0 \left[1 - |0\rangle\rangle\langle\langle\tilde{0}|\right] = L_0$, 则式 (F.8) 可以表示为

$$\tilde{Q}L_0\tilde{Q}|0(\chi)\rangle\rangle = [\lambda_0(\chi) - \Delta L(\chi)]|0(\chi)\rangle\rangle, \tag{F.9}$$

在式 (F.9) 中 $L_0$ 是奇异性的, 因而, 在算符 $\tilde{Q}$ 张开的子空间中引入赝逆算符:

$$\tilde{R} = \tilde{Q}(L_0)^{-1}\tilde{Q}, \tag{F.10}$$

将式 (F.10) 的赝逆算符作用到式 (F.9) 两边可得

$$\tilde{Q}|0(\chi)\rangle\rangle = \tilde{R}[\lambda_0(\chi) - \Delta L(\chi)]|0(\chi)\rangle\rangle, \tag{F.11}$$

式 (F.11) 和式 (F.7) 组成一个封闭方程, 将式 (F.11) 代入式 (F.7), 考虑三阶的情况可得

$$\begin{aligned}
&|0(\chi)\rangle\rangle \\
=&|0\rangle\rangle+\tilde{R}[\lambda_0(\chi)-\Delta L(\chi)]|0\rangle\rangle \\
&+\tilde{R}[\lambda_0(\chi)-\Delta L(\chi)]\tilde{R}[\lambda_0(\chi)-\Delta L(\chi)]|0\rangle\rangle \\
&+\tilde{R}[\lambda_0(\chi)-\Delta L(\chi)]\tilde{R}[\lambda_0(\chi)-\Delta L(\chi)]\tilde{R}[\lambda_0(\chi)-\Delta L(\chi)]|0\rangle\rangle+\cdots
\end{aligned} \tag{F.12}$$

将式 (F.12) 代入式 (F.6) 可得

$$\begin{aligned}
\lambda_0(\chi)&=\langle\langle\tilde{0}|\,\Delta L(\chi)\,|0(\chi)\rangle\rangle \\
&=\langle\langle\tilde{0}|\,\Delta L(\chi)\,|0\rangle\rangle+\langle\langle\tilde{0}|\,\Delta L(\chi)\,\tilde{R}[\lambda_0(\chi)-\Delta L(\chi)]|0\rangle\rangle \\
&\quad+\langle\langle\tilde{0}|\,\Delta L(\chi)\,\tilde{R}[\lambda_0(\chi)-\Delta L(\chi)]\tilde{R}[\lambda_0(\chi)-\Delta L(\chi)]|0\rangle\rangle \\
&\quad+\langle\langle\tilde{0}|\,\Delta L(\chi)\,\tilde{R}[\lambda_0(\chi)-\Delta L(\chi)]\tilde{R}[\lambda_0(\chi)-\Delta L(\chi)] \\
&\quad\times\tilde{R}[\lambda_0(\chi)-\Delta L(\chi)]|0\rangle\rangle+\cdots
\end{aligned} \tag{F.13}$$

将式 (F.2) 和式 (F.3) 代入上式, 并将其按照 (i$\chi$) 的幂次整理可得

$$C_1=\langle\langle\tilde{0}|\,L_1\,|0\rangle\rangle, \tag{F.14}$$

$$C_2=\langle\langle\tilde{0}|\,L_2\,|0\rangle\rangle-2\,\langle\langle\tilde{0}|\,L_1\tilde{R}L_1\,|0\rangle\rangle, \tag{F.15}$$

$$\begin{aligned}
C_3=&\langle\langle\tilde{0}|\,L_3\,|0\rangle\rangle-3\left[\langle\langle\tilde{0}|\,L_1\tilde{R}L_2\,|0\rangle\rangle+\langle\langle\tilde{0}|\,L_2\tilde{R}L_1\,|0\rangle\rangle\right] \\
&-6\left[\langle\langle\tilde{0}|\,L_1\tilde{R}C_1\tilde{R}L_1\,|0\rangle\rangle-\langle\langle\tilde{0}|\,L_1\tilde{R}L_1\tilde{R}L_1\,|0\rangle\rangle\right],
\end{aligned} \tag{F.16}$$

$$\begin{aligned}
C_4=&\langle\langle\tilde{0}|\,L_4\,|0\rangle\rangle-6\,\langle\langle\tilde{0}|\,L_2\tilde{R}L_2\,|0\rangle\rangle-4\,\langle\langle\tilde{0}|\,L_1\tilde{R}L_3\,|0\rangle\rangle-4\,\langle\langle\tilde{0}|\,L_3\tilde{R}L_1\,|0\rangle\rangle \\
&-12\,\langle\langle\tilde{0}|\,L_1\tilde{R}C_2\tilde{R}L_1\,|0\rangle\rangle+12\,\langle\langle\tilde{0}|\,L_1\tilde{R}L_2\tilde{R}L_1\,|0\rangle\rangle-12\,\langle\langle\tilde{0}|\,L_1\tilde{R}C_1\tilde{R}L_2\,|0\rangle\rangle \\
&+12\,\langle\langle\tilde{0}|\,L_1\tilde{R}L_1\tilde{R}L_2\,|0\rangle\rangle-12\,\langle\langle\tilde{0}|\,L_2\tilde{R}C_1\tilde{R}L_1\,|0\rangle\rangle+12\,\langle\langle\tilde{0}|\,L_2\tilde{R}L_1\tilde{R}L_1\,|0\rangle\rangle \\
&-24\,\langle\langle\tilde{0}|\,L_1\tilde{R}C_1\tilde{R}C_1\tilde{R}L_1\,|0\rangle\rangle+24\,\langle\langle\tilde{0}|\,L_1\tilde{R}L_1\tilde{R}C_1\tilde{R}L_1\,|0\rangle\rangle \\
&+24\,\langle\langle\tilde{0}|\,L_1\tilde{R}C_1\tilde{R}L_1\tilde{R}L_1\,|0\rangle\rangle-24\,\langle\langle\tilde{0}|\,L_1\tilde{R}L_1\tilde{R}L_1\tilde{R}L_1\,|0\rangle\rangle.
\end{aligned} \tag{F.17}$$

将式 (F.14) 代入式 (F.16), 并考虑超算符 $\tilde{P}=|0\rangle\rangle\,\langle\langle\tilde{0}|$, 可得

$$\begin{aligned}
C_3=&\langle\langle\tilde{0}|\,L_3\,|0\rangle\rangle-3\left[\langle\langle\tilde{0}|\,L_1\tilde{R}L_2\,|0\rangle\rangle+\langle\langle\tilde{0}|\,L_2\tilde{R}L_1\,|0\rangle\rangle\right] \\
&-6\left[\langle\langle\tilde{0}|\,L_1\tilde{R}\tilde{R}L_1\,|0\rangle\rangle\,\langle\langle\tilde{0}|\,L_1\,|0\rangle\rangle-\langle\langle\tilde{0}|\,L_1\tilde{R}L_1\tilde{R}L_1\,|0\rangle\rangle\right]
\end{aligned}$$

$$
\begin{aligned}
&= \langle\langle \tilde{0} |\, L_3 \,| 0 \rangle\rangle - 3 \langle\langle \tilde{0} | \left( L_1 \tilde{R} L_2 + L_2 \tilde{R} L_1 \right) | 0 \rangle\rangle \\
&\quad - 6 \langle\langle \tilde{0} |\, L_1 \tilde{R} \left( \tilde{R} L_1 \tilde{P} - L_1 \tilde{R} \right) L_1 \,| 0 \rangle\rangle ,
\end{aligned}
\tag{F.18}
$$

同理, 将式 (F.14) 和式 (F.15) 代入式 (F.17), 可得

$$
\begin{aligned}
C_4 &= \langle\langle \tilde{0} |\, L_4 \,| 0 \rangle\rangle - 6 \langle\langle \tilde{0} |\, L_2 \tilde{R} L_2 \,| 0 \rangle\rangle - 4 \langle\langle \tilde{0} | \left( L_1 \tilde{R} L_3 + L_3 \tilde{R} L_1 \right) | 0 \rangle\rangle \\
&\quad - 12 \langle\langle \tilde{0} |\, L_1 \tilde{R} \tilde{R} L_1 \,| 0 \rangle\rangle \langle\langle \tilde{0} |\, L_2 \,| 0 \rangle\rangle + 24 \langle\langle \tilde{0} |\, L_1 \tilde{R} \tilde{R} L_1 \,| 0 \rangle\rangle \langle\langle \tilde{0} |\, L_1 \tilde{R} L_1 \,| 0 \rangle\rangle \\
&\quad + 12 \langle\langle \tilde{0} |\, L_1 \tilde{R} L_2 \tilde{R} L_1 \,| 0 \rangle\rangle - 12 \langle\langle \tilde{0} |\, L_1 \tilde{R} \tilde{R} L_2 \,| 0 \rangle\rangle \langle\langle \tilde{0} |\, L_1 \,| 0 \rangle\rangle \\
&\quad + 12 \langle\langle \tilde{0} |\, L_1 \tilde{R} L_1 \tilde{R} L_2 \,| 0 \rangle\rangle - 12 \langle\langle \tilde{0} |\, L_2 \tilde{R} \tilde{R} L_1 \,| 0 \rangle\rangle \langle\langle \tilde{0} |\, L_1 \,| 0 \rangle\rangle \\
&\quad + 12 \langle\langle \tilde{0} |\, L_2 \tilde{R} L_1 \tilde{R} L_1 \,| 0 \rangle\rangle - 24 \langle\langle \tilde{0} |\, L_1 \tilde{R} \tilde{R} \tilde{R} L_1 \,| 0 \rangle\rangle \langle\langle \tilde{0} |\, L_1 \,| 0 \rangle\rangle \langle\langle \tilde{0} |\, L_1 \,| 0 \rangle\rangle \\
&\quad + 24 \langle\langle \tilde{0} |\, L_1 \tilde{R} L_1 \tilde{R} \tilde{R} L_1 \,| 0 \rangle\rangle \langle\langle \tilde{0} |\, L_1 \,| 0 \rangle\rangle - 24 \langle\langle \tilde{0} |\, L_1 \tilde{R} L_1 \tilde{R} L_1 \tilde{R} L_1 \,| 0 \rangle\rangle \\
&\quad + 24 \langle\langle \tilde{0} |\, L_1 \tilde{R} \tilde{R} L_1 \tilde{R} L_1 \,| 0 \rangle\rangle \langle\langle \tilde{0} |\, L_1 \,| 0 \rangle\rangle ,
\end{aligned}
\tag{F.19}
$$

考虑超算符 $\tilde{P} = | 0 \rangle\rangle \langle\langle \tilde{0} |$, 式 (F.19) 可简化为

$$
\begin{aligned}
C_4 &= \langle\langle \tilde{0} |\, L_4 \,| 0 \rangle\rangle - 6 \langle\langle \tilde{0} |\, L_2 \tilde{R} L_2 \,| 0 \rangle\rangle \\
&\quad - 4 \langle\langle \tilde{0} | \left( L_1 \tilde{R} L_3 + L_3 \tilde{R} L_1 \right) | 0 \rangle\rangle - 12 \langle\langle \tilde{0} |\, L_1 \tilde{R} \left( \tilde{R} L_2 \tilde{P} - L_2 \tilde{R} \right) L_1 \,| 0 \rangle\rangle \\
&\quad - 12 \langle\langle \tilde{0} |\, L_1 \tilde{R} \left( \tilde{R} L_1 \tilde{P} - L_1 \tilde{R} \right) L_2 \,| 0 \rangle\rangle - 12 \langle\langle \tilde{0} |\, L_2 \tilde{R} \left( \tilde{R} L_1 \tilde{P} - L_1 \tilde{R} \right) L_1 \,| 0 \rangle\rangle \\
&\quad - 24 \langle\langle \tilde{0} |\, L_1 \tilde{R} \left( \tilde{R} \tilde{R} L_1 \tilde{P} L_1 \tilde{P} - \tilde{R} L_1 \tilde{P} L_1 \tilde{R} - L_1 \tilde{R} \tilde{R} L_1 \tilde{P} \right. \\
&\quad \left. - \tilde{R} L_1 \tilde{R} L_1 \tilde{P} + L_1 \tilde{R} L_1 \tilde{R} \right) L_1 \,| 0 \rangle\rangle .
\end{aligned}
\tag{F.20}
$$

式 (F.14)、(F.15)、(F.18) 和 (F.20) 即为开放量子系统电流前四阶累积矩的表达式.

# 附录 G　共隧穿过程的条件性约化密度矩阵

在本附录中, 将给出式 (4.46)~式 (4.49) 对应的条件性约化密度矩阵的表达式. 式 (4.46) 对应的条件性约化密度矩阵可以表示为如下四项:

$$
\begin{aligned}
&\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t} \rho_{\mathrm{QS,I}}(t) \Big|_{\text{fourth-order}} \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t} \Big|_{02,\mathrm{con}} \Big|_{01} \\
&= \sum_{ijkl} \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \int_{t_0}^{t_2} \mathrm{d}t_3 \\
&\quad \times \Big[ C_{\mathrm{L}02}^{(-)} C_{\mathrm{L}31}^{(-)} d_{i,0}^{\dagger} d_{k,2} d_{j,1} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\, d_{l,3}^{\dagger} + C_{\mathrm{R}02}^{(-)} C_{\mathrm{L}31}^{(-)} d_{i,0}^{\dagger} d_{k,2} d_{j,1} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\, d_{l,3}^{\dagger}
\end{aligned}
$$

$$
\begin{aligned}
&+C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(-)}d_{i,0}d_{k,2}^{\dagger}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{l,3}^{\dagger}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(-)}d_{i,0}d_{k,2}^{\dagger}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{l,3}^{\dagger}\\
&+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(-)}d_{i,0}^{\dagger}d_{k,2}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{l,3}^{\dagger}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(-)}d_{i,0}^{\dagger}d_{k,2}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{l,3}^{\dagger}\\
&+C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(-)}d_{i,0}d_{k,2}^{\dagger}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{l,3}^{\dagger}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(-)}d_{i,0}d_{k,2}^{\dagger}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{l,3}^{\dagger}\\
&+C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(+)}d_{i,0}^{\dagger}d_{k,2}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{l,3}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(+)}d_{i,0}^{\dagger}d_{k,2}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{l,3}\\
&+C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(+)}d_{i,0}d_{k,2}^{\dagger}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{l,3}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(+)}d_{i,0}d_{k,2}^{\dagger}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{l,3}\\
&+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(+)}d_{i,0}^{\dagger}d_{k,2}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{l,3}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(+)}d_{i,0}^{\dagger}d_{k,2}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{l,3}\\
&\left.+C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(+)}d_{i,0}d_{k,2}^{\dagger}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{l,3}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(+)}d_{i,0}d_{k,2}^{\dagger}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{l,3}\right]\\
&+\mathrm{H.c.},
\end{aligned}
\tag{G.1}
$$

$$
\begin{aligned}
&\left.\left.\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\right|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\right|_{02,\mathrm{con}}\Big|_{02}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\Big[-C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(-)}d_{i,0}^{\dagger}d_{j,1}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{l,3}^{\dagger}-C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(-)}d_{i,0}^{\dagger}d_{j,1}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{l,3}^{\dagger}\\
&-C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(-)}d_{i,0}d_{j,1}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{l,3}^{\dagger}-C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(-)}d_{i,0}d_{j,1}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{l,3}^{\dagger}\\
&-C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(-)}d_{i,0}^{\dagger}d_{j,1}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{l,3}^{\dagger}-C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(-)}d_{i,0}^{\dagger}d_{j,1}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{l,3}^{\dagger}\\
&-C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(-)}d_{i,0}d_{j,1}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{l,3}^{\dagger}-C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(-)}d_{i,0}d_{j,1}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{l,3}^{\dagger}\\
&-C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(+)}d_{i,0}^{\dagger}d_{j,1}^{\dagger}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{l,3}-C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(+)}d_{i,0}^{\dagger}d_{j,1}^{\dagger}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{l,3}\\
&-C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(+)}d_{i,0}d_{j,1}^{\dagger}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{l,3}-C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(+)}d_{i,0}d_{j,1}^{\dagger}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{l,3}\\
&-C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(+)}d_{i,0}^{\dagger}d_{j,1}^{\dagger}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{l,3}-C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(+)}d_{i,0}^{\dagger}d_{j,1}^{\dagger}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{l,3}\\
&\left.-C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(+)}d_{i,0}d_{j,1}^{\dagger}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{l,3}-C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(+)}d_{i,0}d_{j,1}^{\dagger}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{l,3}\right]\\
&+\mathrm{H.c.},
\end{aligned}
\tag{G.2}
$$

$$
\begin{aligned}
&\left.\left.\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\right|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\right|_{02,\mathrm{con}}\Big|_{03}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\Big[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(-)}d_{j,1}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-2,n_{\mathrm{R}})}(t)\,d_{l,3}^{\dagger}d_{i,0}^{\dagger}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(-)}d_{j,1}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}-1)}(t)\,d_{l,3}^{\dagger}d_{i,0}^{\dagger}\\
&+C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(+)}d_{j,1}^{\dagger}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\,d_{l,3}d_{i,0}^{\dagger}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(+)}d_{j,1}^{\dagger}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}+1)}(t)\,d_{l,3}d_{i,0}^{\dagger}\\
&+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(-)}d_{j,1}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}-1)}(t)\,d_{l,3}^{\dagger}d_{i,0}^{\dagger}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(-)}d_{j,1}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-2)}(t)\,d_{l,3}^{\dagger}d_{i,0}^{\dagger}\\
&+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(+)}d_{j,1}^{\dagger}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}-1)}(t)\,d_{l,3}d_{i,0}^{\dagger}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(+)}d_{j,1}^{\dagger}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\,d_{l,3}d_{i,0}^{\dagger}
\end{aligned}
$$

$$
\begin{aligned}
&+C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(-)}d_{j,1}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\,d_{l,3}^{\dagger}d_{i,0}+C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(-)}d_{j,1}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}-1)}(t)\,d_{l,3}^{\dagger}d_{i,0}\\
&+C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(+)}d_{j,1}^{\dagger}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+2,n_{\mathrm{R}})}(t)\,d_{l,3}d_{i,0}+C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(+)}d_{j,1}^{\dagger}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}+1)}(t)\,d_{l,3}d_{i,0}\\
&+C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(-)}d_{j,1}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}+1)}(t)\,d_{l,3}^{\dagger}d_{i,0}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(-)}d_{j,1}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\,d_{l,3}^{\dagger}d_{i,0}\\
&\left.+C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(+)}d_{j,1}^{\dagger}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}+1)}(t)\,d_{l,3}d_{i,0}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(+)}d_{j,1}^{\dagger}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+2)}(t)\,d_{l,3}d_{i,0}\right]\\
&+\mathrm{H.c.},
\end{aligned}
\tag{G.3}
$$

$$
\begin{aligned}
&\left.\left.\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\right|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\right|_{02,\mathrm{con}}\Big|_{04}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\Big[-C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(-)}d_{k,2}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-2,n_{\mathrm{R}})}(t)\,d_{l,3}^{\dagger}d_{i,0}^{\dagger}-C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(-)}d_{k,2}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}-1)}(t)\,d_{l,3}^{\dagger}d_{i,0}^{\dagger}\\
&-C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(+)}d_{k,2}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\,d_{l,3}d_{i,0}^{\dagger}-C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(+)}d_{k,2}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}+1)}(t)\,d_{l,3}d_{i,0}^{\dagger}\\
&-C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(-)}d_{k,2}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}-1)}(t)\,d_{l,3}^{\dagger}d_{i,0}^{\dagger}-C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(-)}d_{k,2}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-2)}(t)\,d_{l,3}^{\dagger}d_{i,0}^{\dagger}\\
&-C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(+)}d_{k,2}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}-1)}(t)\,d_{l,3}d_{i,0}^{\dagger}-C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(+)}d_{k,2}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\,d_{l,3}d_{i,0}^{\dagger}\\
&-C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(-)}d_{k,2}^{\dagger}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\,d_{l,3}^{\dagger}d_{i,0}-C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(-)}d_{k,2}^{\dagger}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}-1)}(t)\,d_{l,3}^{\dagger}d_{i,0}\\
&-C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(+)}d_{k,2}^{\dagger}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+2,n_{\mathrm{R}})}(t)\,d_{l,3}d_{i,0}-C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(+)}d_{k,2}^{\dagger}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}+1)}(t)\,d_{l,3}d_{i,0}\\
&-C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(-)}d_{k,2}^{\dagger}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}+1)}(t)\,d_{l,3}^{\dagger}d_{i,0}-C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(-)}d_{k,2}^{\dagger}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\,d_{l,3}^{\dagger}d_{i,0}\\
&\left.-C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(+)}d_{k,2}^{\dagger}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}+1)}(t)\,d_{l,3}d_{i,0}-C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(+)}d_{k,2}^{\dagger}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+2)}(t)\,d_{l,3}d_{i,0}\right]\\
&+\mathrm{H.c.}.
\end{aligned}
\tag{G.4}
$$

式 (4.47) 对应的条件性约化密度矩阵可以表示为如下四项：

$$
\begin{aligned}
&\left.\left.\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\right|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\right|_{03,\mathrm{con}}\Big|_{01}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\Big[C_{03}^{(-)}C_{12}^{(-)}d_{i,0}^{\dagger}d_{j,1}^{\dagger}d_{k,2}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)+C_{03}^{(-)}C_{12}^{(+)}d_{i,0}^{\dagger}d_{j,1}d_{k,2}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\\
&\left.+C_{03}^{(+)}C_{12}^{(-)}d_{i,0}d_{j,1}^{\dagger}d_{k,2}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)+C_{03}^{(+)}C_{12}^{(+)}d_{i,0}d_{j,1}d_{k,2}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\right]\\
&+\mathrm{H.c.},
\end{aligned}
\tag{G.5}
$$

$$
\left.\left.\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\right|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\right|_{03,\mathrm{con}}\Big|_{02}
$$

$$
\begin{aligned}
&= \sum_{ijkl} \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \int_{t_0}^{t_2} \mathrm{d}t_3 \\
&\quad \times \Big[ -C_{03}^{(-)} C_{12}^{(-)} d_{i,0}^{\dagger} d_{l,3} d_{j,1}^{\dagger} d_{k,2} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t) - C_{03}^{(-)} C_{12}^{(+)} d_{i,0}^{\dagger} d_{l,3} d_{j,1} d_{k,2}^{\dagger} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t) \\
&\quad -C_{03}^{(+)} C_{12}^{(-)} d_{i,0} d_{l,3}^{\dagger} d_{j,1}^{\dagger} d_{k,2} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t) - C_{03}^{(+)} C_{12}^{(+)} d_{i,0} d_{l,3}^{\dagger} d_{j,1} d_{k,2}^{\dagger} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t) \Big] \\
&\quad + \mathrm{H.c.},
\end{aligned} \tag{G.6}
$$

$$
\begin{aligned}
&\quad \mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t} \rho_{\mathrm{QS,I}}(t)\Big|_{\text{fourth-order}} \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{03,\mathrm{con}}\Big|_{03} \\
&= \sum_{ijkl} \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \int_{t_0}^{t_2} \mathrm{d}t_3 \\
&\quad \times \Big[ C_{\mathrm{L}03}^{(-)} C_{\mathrm{L}12}^{(-)} d_{l,3} d_{j,1}^{\dagger} d_{k,2} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\, d_{i,0}^{\dagger} + C_{\mathrm{L}03}^{(-)} C_{\mathrm{R}12}^{(-)} d_{l,3} d_{j,1}^{\dagger} d_{k,2} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\, d_{i,0}^{\dagger} \\
&\quad + C_{\mathrm{L}03}^{(-)} C_{\mathrm{L}12}^{(+)} d_{l,3} d_{j,1} d_{k,2}^{\dagger} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\, d_{i,0}^{\dagger} + C_{\mathrm{L}03}^{(-)} C_{\mathrm{R}12}^{(+)} d_{l,3} d_{j,1} d_{k,2}^{\dagger} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\, d_{i,0}^{\dagger} \\
&\quad + C_{\mathrm{R}03}^{(-)} C_{\mathrm{L}12}^{(-)} d_{l,3} d_{j,1}^{\dagger} d_{k,2} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\, d_{i,0}^{\dagger} + C_{\mathrm{R}03}^{(-)} C_{\mathrm{R}12}^{(-)} d_{l,3} d_{j,1}^{\dagger} d_{k,2} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\, d_{i,0}^{\dagger} \\
&\quad + C_{\mathrm{R}03}^{(-)} C_{\mathrm{L}12}^{(+)} d_{l,3} d_{j,1} d_{k,2}^{\dagger} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\, d_{i,0}^{\dagger} + C_{\mathrm{R}03}^{(-)} C_{\mathrm{R}12}^{(+)} d_{l,3} d_{j,1} d_{k,2}^{\dagger} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\, d_{i,0}^{\dagger} \\
&\quad + C_{\mathrm{L}03}^{(+)} C_{\mathrm{L}12}^{(-)} d_{l,3}^{\dagger} d_{j,1}^{\dagger} d_{k,2} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\, d_{i,0} + C_{\mathrm{L}03}^{(+)} C_{\mathrm{R}12}^{(-)} d_{l,3}^{\dagger} d_{j,1}^{\dagger} d_{k,2} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\, d_{i,0} \\
&\quad + C_{\mathrm{L}03}^{(+)} C_{\mathrm{L}12}^{(+)} d_{l,3}^{\dagger} d_{j,1} d_{k,2}^{\dagger} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\, d_{i,0} + C_{\mathrm{L}03}^{(+)} C_{\mathrm{R}12}^{(+)} d_{l,3}^{\dagger} d_{j,1} d_{k,2}^{\dagger} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\, d_{i,0} \\
&\quad + C_{\mathrm{R}03}^{(+)} C_{\mathrm{L}12}^{(-)} d_{l,3}^{\dagger} d_{j,1}^{\dagger} d_{k,2} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\, d_{i,0} + C_{\mathrm{R}03}^{(+)} C_{\mathrm{R}12}^{(-)} d_{l,3}^{\dagger} d_{j,1}^{\dagger} d_{k,2} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\, d_{i,0} \\
&\quad + C_{\mathrm{R}03}^{(+)} C_{\mathrm{L}12}^{(+)} d_{l,3}^{\dagger} d_{j,1} d_{k,2}^{\dagger} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\, d_{i,0} + C_{\mathrm{R}03}^{(+)} C_{\mathrm{R}12}^{(+)} d_{l,3}^{\dagger} d_{j,1} d_{k,2}^{\dagger} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\, d_{i,0} \Big] \\
&\quad + \mathrm{H.c.},
\end{aligned} \tag{G.7}
$$

$$
\begin{aligned}
&\quad \mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t} \rho_{\mathrm{QS,I}}(t)\Big|_{\text{fourth-order}} \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{03,\mathrm{con}}\Big|_{04} \\
&= \sum_{ijkl} \int_{t_0}^{t} \mathrm{d}t_1 \int_{t_0}^{t_1} \mathrm{d}t_2 \int_{t_0}^{t_2} \mathrm{d}t_3 \\
&\quad \times \Big[ -C_{\mathrm{L}03}^{(-)} C_{\mathrm{L}12}^{(-)} d_{j,1}^{\dagger} d_{k,2} d_{l,3} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\, d_{i,0}^{\dagger} - C_{\mathrm{L}03}^{(-)} C_{\mathrm{R}12}^{(-)} d_{j,1}^{\dagger} d_{k,2} d_{l,3} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\, d_{i,0}^{\dagger} \\
&\quad - C_{\mathrm{L}03}^{(-)} C_{\mathrm{L}12}^{(+)} d_{j,1} d_{k,2}^{\dagger} d_{l,3} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\, d_{i,0}^{\dagger} - C_{\mathrm{L}03}^{(-)} C_{\mathrm{R}12}^{(+)} d_{j,1} d_{k,2}^{\dagger} d_{l,3} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\, d_{i,0}^{\dagger} \\
&\quad - C_{\mathrm{R}03}^{(-)} C_{\mathrm{L}12}^{(-)} d_{j,1}^{\dagger} d_{k,2} d_{l,3} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\, d_{i,0}^{\dagger} - C_{\mathrm{R}03}^{(-)} C_{\mathrm{R}12}^{(-)} d_{j,1}^{\dagger} d_{k,2} d_{l,3} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\, d_{i,0}^{\dagger} \\
&\quad - C_{\mathrm{R}03}^{(-)} C_{\mathrm{L}12}^{(+)} d_{j,1} d_{k,2}^{\dagger} d_{l,3} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\, d_{i,0}^{\dagger} - C_{\mathrm{R}03}^{(-)} C_{\mathrm{R}12}^{(+)} d_{j,1} d_{k,2}^{\dagger} d_{l,3} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\, d_{i,0}^{\dagger} \\
&\quad - C_{\mathrm{L}03}^{(+)} C_{\mathrm{L}12}^{(-)} d_{j,1}^{\dagger} d_{k,2} d_{l,3}^{\dagger} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\, d_{i,0} - C_{\mathrm{L}03}^{(+)} C_{\mathrm{R}12}^{(-)} d_{j,1}^{\dagger} d_{k,2} d_{l,3}^{\dagger} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\, d_{i,0} \\
&\quad - C_{\mathrm{L}03}^{(+)} C_{\mathrm{L}12}^{(+)} d_{j,1} d_{k,2}^{\dagger} d_{l,3}^{\dagger} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\, d_{i,0} - C_{\mathrm{L}03}^{(+)} C_{\mathrm{R}12}^{(+)} d_{j,1} d_{k,2}^{\dagger} d_{l,3}^{\dagger} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\, d_{i,0} \\
&\quad - C_{\mathrm{R}03}^{(+)} C_{\mathrm{L}12}^{(-)} d_{j,1}^{\dagger} d_{k,2} d_{l,3}^{\dagger} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\, d_{i,0} - C_{\mathrm{R}03}^{(+)} C_{\mathrm{R}12}^{(-)} d_{j,1}^{\dagger} d_{k,2} d_{l,3}^{\dagger} \rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\, d_{i,0}
\end{aligned}
$$

$$
\begin{aligned}
&-C_{\mathrm{R}03}^{(+)}C_{\mathrm{L}12}^{(+)}d_{j,1}d_{k,2}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{i,0}-C_{\mathrm{R}03}^{(+)}C_{\mathrm{R}12}^{(+)}d_{j,1}d_{k,2}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{i,0}\Big]\\
&+\mathrm{H.c.}.
\end{aligned}
\tag{G.8}
$$

式 (4.48) 对应的条件性约化密度矩阵可以表示为如下四项：

$$
\begin{aligned}
&\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\Big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{04,\mathrm{con}}\Big|_{01}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\Big[C_{\mathrm{L}03}^{(-)}C_{\mathrm{L}12}^{(-)}d_{i,0}^{\dagger}d_{l,3}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{j,1}^{\dagger}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{L}12}^{(-)}d_{i,0}^{\dagger}d_{l,3}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{j,1}^{\dagger}\\
&+C_{\mathrm{L}03}^{(+)}C_{\mathrm{L}12}^{(-)}d_{i,0}d_{l,3}^{\dagger}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{j,1}^{\dagger}+C_{\mathrm{R}03}^{(+)}C_{\mathrm{L}12}^{(-)}d_{i,0}d_{l,3}^{\dagger}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{j,1}^{\dagger}\\
&+C_{\mathrm{L}03}^{(-)}C_{\mathrm{R}12}^{(-)}d_{i,0}^{\dagger}d_{l,3}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{j,1}^{\dagger}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{R}12}^{(-)}d_{i,0}^{\dagger}d_{l,3}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{j,1}^{\dagger}\\
&+C_{\mathrm{L}03}^{(+)}C_{\mathrm{R}12}^{(-)}d_{i,0}d_{l,3}^{\dagger}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{j,1}^{\dagger}+C_{\mathrm{R}03}^{(+)}C_{\mathrm{R}12}^{(-)}d_{i,0}d_{l,3}^{\dagger}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{j,1}^{\dagger}\\
&+C_{\mathrm{L}03}^{(-)}C_{\mathrm{L}12}^{(+)}d_{i,0}^{\dagger}d_{l,3}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{j,1}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{L}12}^{(+)}d_{i,0}^{\dagger}d_{l,3}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{j,1}\\
&+C_{\mathrm{L}03}^{(+)}C_{\mathrm{L}12}^{(+)}d_{i,0}d_{l,3}^{\dagger}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{j,1}+C_{\mathrm{R}03}^{(+)}C_{\mathrm{L}12}^{(+)}d_{i,0}d_{l,3}^{\dagger}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{j,1}\\
&+C_{\mathrm{L}03}^{(-)}C_{\mathrm{R}12}^{(+)}d_{i,0}^{\dagger}d_{l,3}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{j,1}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{R}12}^{(+)}d_{i,0}^{\dagger}d_{l,3}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{j,1}\\
&+C_{\mathrm{L}03}^{(+)}C_{\mathrm{R}12}^{(+)}d_{i,0}d_{l,3}^{\dagger}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{j,1}+C_{\mathrm{R}03}^{(+)}C_{\mathrm{R}12}^{(+)}d_{i,0}d_{l,3}^{\dagger}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{j,1}\Big]\\
&+\mathrm{H.c.},
\end{aligned}
\tag{G.9}
$$

$$
\begin{aligned}
&\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\Big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{04,\mathrm{con}}\Big|_{02}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\Big[-C_{\mathrm{L}03}^{(-)}C_{\mathrm{L}12}^{(-)}d_{i,0}^{\dagger}d_{k,2}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{j,1}^{\dagger}-C_{\mathrm{R}03}^{(-)}C_{\mathrm{L}12}^{(-)}d_{i,0}^{\dagger}d_{k,2}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{j,1}^{\dagger}\\
&-C_{\mathrm{L}03}^{(+)}C_{\mathrm{L}12}^{(-)}d_{i,0}d_{k,2}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{j,1}^{\dagger}-C_{\mathrm{R}03}^{(+)}C_{\mathrm{L}12}^{(-)}d_{i,0}d_{k,2}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{j,1}^{\dagger}\\
&-C_{\mathrm{L}03}^{(-)}C_{\mathrm{R}12}^{(-)}d_{i,0}^{\dagger}d_{k,2}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{j,1}^{\dagger}-C_{\mathrm{R}03}^{(-)}C_{\mathrm{R}12}^{(-)}d_{i,0}^{\dagger}d_{k,2}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{j,1}^{\dagger}\\
&-C_{\mathrm{L}03}^{(+)}C_{\mathrm{R}12}^{(-)}d_{i,0}d_{k,2}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{j,1}^{\dagger}-C_{\mathrm{R}03}^{(+)}C_{\mathrm{R}12}^{(-)}d_{i,0}d_{k,2}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{j,1}^{\dagger}\\
&-C_{\mathrm{L}03}^{(-)}C_{\mathrm{L}12}^{(+)}d_{i,0}^{\dagger}d_{k,2}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{j,1}-C_{\mathrm{R}03}^{(-)}C_{\mathrm{L}12}^{(+)}d_{i,0}^{\dagger}d_{k,2}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{j,1}\\
&-C_{\mathrm{L}03}^{(+)}C_{\mathrm{L}12}^{(+)}d_{i,0}d_{k,2}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{j,1}-C_{\mathrm{R}03}^{(+)}C_{\mathrm{L}12}^{(+)}d_{i,0}d_{k,2}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{j,1}\\
&-C_{\mathrm{L}03}^{(-)}C_{\mathrm{R}12}^{(+)}d_{i,0}^{\dagger}d_{k,2}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{j,1}-C_{\mathrm{R}03}^{(-)}C_{\mathrm{R}12}^{(+)}d_{i,0}^{\dagger}d_{k,2}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{j,1}\\
&-C_{\mathrm{L}03}^{(+)}C_{\mathrm{R}12}^{(+)}d_{i,0}d_{k,2}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{j,1}-C_{\mathrm{R}03}^{(+)}C_{\mathrm{R}12}^{(+)}d_{i,0}d_{k,2}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{j,1}\Big]\\
&+\mathrm{H.c.},
\end{aligned}
\tag{G.10}
$$

$$
\begin{aligned}
&\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{04,\mathrm{con}}\Big|_{03}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\Big[C_{\mathrm{L}03}^{(-)}C_{\mathrm{L}12}^{(-)}d_{k,2}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-2,n_{\mathrm{R}})}\left(t\right)d_{j,1}^{\dagger}d_{i,0}^{\dagger}+C_{\mathrm{L}03}^{(-)}C_{\mathrm{R}12}^{(-)}d_{k,2}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}-1)}\left(t\right)d_{j,1}^{\dagger}d_{i,0}^{\dagger}\\
&+C_{\mathrm{L}03}^{(-)}C_{\mathrm{L}12}^{(+)}d_{k,2}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}\left(t\right)d_{j,1}d_{i,0}^{\dagger}+C_{\mathrm{L}03}^{(-)}C_{\mathrm{R}12}^{(+)}d_{k,2}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}+1)}\left(t\right)d_{j,1}d_{i,0}^{\dagger}\\
&+C_{\mathrm{R}03}^{(-)}C_{\mathrm{L}12}^{(-)}d_{k,2}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}-1)}\left(t\right)d_{j,1}^{\dagger}d_{i,0}^{\dagger}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{R}12}^{(-)}d_{k,2}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-2)}\left(t\right)d_{j,1}^{\dagger}d_{i,0}^{\dagger}\\
&+C_{\mathrm{R}03}^{(-)}C_{\mathrm{L}12}^{(+)}d_{k,2}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}-1)}\left(t\right)d_{j,1}d_{i,0}^{\dagger}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{R}12}^{(+)}d_{k,2}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}\left(t\right)d_{j,1}d_{i,0}^{\dagger}\\
&+C_{\mathrm{L}03}^{(+)}C_{\mathrm{L}12}^{(-)}d_{k,2}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}\left(t\right)d_{j,1}^{\dagger}d_{i,0}+C_{\mathrm{L}03}^{(+)}C_{\mathrm{R}12}^{(-)}d_{k,2}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}-1)}\left(t\right)d_{j,1}^{\dagger}d_{i,0}\\
&+C_{\mathrm{L}03}^{(+)}C_{\mathrm{L}12}^{(+)}d_{k,2}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+2,n_{\mathrm{R}})}\left(t\right)d_{j,1}d_{i,0}+C_{\mathrm{L}03}^{(+)}C_{\mathrm{R}12}^{(+)}d_{k,2}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}+1)}\left(t\right)d_{j,1}d_{i,0}\\
&+C_{\mathrm{R}03}^{(+)}C_{\mathrm{L}12}^{(-)}d_{k,2}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}+1)}\left(t\right)d_{j,1}^{\dagger}d_{i,0}+C_{\mathrm{R}03}^{(+)}C_{\mathrm{R}12}^{(-)}d_{k,2}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}\left(t\right)d_{j,1}^{\dagger}d_{i,0}\\
&+C_{\mathrm{R}03}^{(+)}C_{\mathrm{L}12}^{(+)}d_{k,2}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}+1)}\left(t\right)d_{j,1}d_{i,0}+C_{\mathrm{R}03}^{(+)}C_{\mathrm{R}12}^{(+)}d_{k,2}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+2)}\left(t\right)d_{j,1}d_{i,0}\Big]\\
&+\mathrm{H.c.},
\end{aligned}
\tag{G.11}
$$

$$
\begin{aligned}
&\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{04,\mathrm{con}}\Big|_{04}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\Big[-C_{\mathrm{L}03}^{(-)}C_{\mathrm{L}12}^{(-)}d_{l,3}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-2,n_{\mathrm{R}})}\left(t\right)d_{j,1}^{\dagger}d_{i,0}^{\dagger}-C_{\mathrm{L}03}^{(-)}C_{\mathrm{R}12}^{(-)}d_{l,3}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}-1)}\left(t\right)d_{j,1}^{\dagger}d_{i,0}^{\dagger}\\
&-C_{\mathrm{L}03}^{(-)}C_{\mathrm{L}12}^{(+)}d_{l,3}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}\left(t\right)d_{j,1}d_{i,0}^{\dagger}-C_{\mathrm{L}03}^{(-)}C_{\mathrm{R}12}^{(+)}d_{l,3}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}+1)}\left(t\right)d_{j,1}d_{i,0}^{\dagger}\\
&-C_{\mathrm{R}03}^{(-)}C_{\mathrm{L}12}^{(-)}d_{l,3}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}-1)}\left(t\right)d_{j,1}^{\dagger}d_{i,0}^{\dagger}-C_{\mathrm{R}03}^{(-)}C_{\mathrm{R}12}^{(-)}d_{l,3}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-2)}\left(t\right)d_{j,1}^{\dagger}d_{i,0}^{\dagger}\\
&-C_{\mathrm{R}03}^{(-)}C_{\mathrm{L}12}^{(+)}d_{l,3}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}-1)}\left(t\right)d_{j,1}d_{i,0}^{\dagger}-C_{\mathrm{R}03}^{(-)}C_{\mathrm{R}12}^{(+)}d_{l,3}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}\left(t\right)d_{j,1}d_{i,0}^{\dagger}\\
&-C_{\mathrm{L}03}^{(+)}C_{\mathrm{L}12}^{(-)}d_{l,3}^{\dagger}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}\left(t\right)d_{j,1}^{\dagger}d_{i,0}-C_{\mathrm{L}03}^{(+)}C_{\mathrm{R}12}^{(-)}d_{l,3}^{\dagger}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}-1)}\left(t\right)d_{j,1}^{\dagger}d_{i,0}\\
&-C_{\mathrm{L}03}^{(+)}C_{\mathrm{L}12}^{(+)}d_{l,3}^{\dagger}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+2,n_{\mathrm{R}})}\left(t\right)d_{j,1}d_{i,0}-C_{\mathrm{L}03}^{(+)}C_{\mathrm{R}12}^{(+)}d_{l,3}^{\dagger}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}+1)}\left(t\right)d_{j,1}d_{i,0}\\
&-C_{\mathrm{R}03}^{(+)}C_{\mathrm{L}12}^{(-)}d_{l,3}^{\dagger}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}+1)}\left(t\right)d_{j,1}^{\dagger}d_{i,0}-C_{\mathrm{R}03}^{(+)}C_{\mathrm{R}12}^{(-)}d_{l,3}^{\dagger}d_{k,2}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}\left(t\right)d_{j,1}^{\dagger}d_{i,0}\\
&-C_{\mathrm{R}03}^{(+)}C_{\mathrm{L}12}^{(+)}d_{l,3}^{\dagger}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}+1)}\left(t\right)d_{j,1}d_{i,0}-C_{\mathrm{R}03}^{(+)}C_{\mathrm{R}12}^{(+)}d_{l,3}^{\dagger}d_{k,2}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+2)}\left(t\right)d_{j,1}d_{i,0}\Big]\\
&+\mathrm{H.c.}.
\end{aligned}
\tag{G.12}
$$

式 (4.49) 对应的条件性约化密度矩阵可以表示为如下四项：

$$
\begin{aligned}
&\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{05,\mathrm{con}}\Big|_{01}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3
\end{aligned}
$$

$$
\begin{aligned}
&\times \Big[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L21}}^{(-)}d_{i,0}^{\dagger}d_{l,3}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{k,2}^{\dagger}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L21}}^{(-)}d_{i,0}^{\dagger}d_{l,3}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{k,2}^{\dagger}\\
&+C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}d_{i,0}d_{l,3}^{\dagger}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{k,2}^{\dagger}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}d_{i,0}d_{l,3}^{\dagger}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{k,2}^{\dagger}\\
&+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R21}}^{(-)}d_{i,0}^{\dagger}d_{l,3}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{k,2}^{\dagger}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R21}}^{(-)}d_{i,0}^{\dagger}d_{l,3}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{k,2}^{\dagger}\\
&+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}d_{i,0}d_{l,3}^{\dagger}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{k,2}^{\dagger}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}d_{i,0}d_{l,3}^{\dagger}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{k,2}^{\dagger}\\
&+C_{\mathrm{L03}}^{(-)}C_{\mathrm{L21}}^{(+)}d_{i,0}^{\dagger}d_{l,3}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{k,2}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L21}}^{(+)}d_{i,0}^{\dagger}d_{l,3}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{k,2}\\
&+C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(+)}d_{i,0}d_{l,3}^{\dagger}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{k,2}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(+)}d_{i,0}d_{l,3}^{\dagger}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{k,2}\\
&+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R21}}^{(+)}d_{i,0}^{\dagger}d_{l,3}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{k,2}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R21}}^{(+)}d_{i,0}^{\dagger}d_{l,3}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{k,2}\\
&+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(+)}d_{i,0}d_{l,3}^{\dagger}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{k,2}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(+)}d_{i,0}d_{l,3}^{\dagger}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{k,2}\Big]\\
&+\mathrm{H.c.},
\end{aligned}
\tag{G.13}
$$

$$
\begin{aligned}
&\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{05,\mathrm{con}}\Big|_{02}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\Big[-C_{\mathrm{L03}}^{(-)}C_{\mathrm{L21}}^{(-)}d_{i,0}^{\dagger}d_{j,1}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{k,2}^{\dagger}-C_{\mathrm{R03}}^{(-)}C_{\mathrm{L21}}^{(-)}d_{i,0}^{\dagger}d_{j,1}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{k,2}^{\dagger}\\
&-C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}d_{i,0}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{k,2}^{\dagger}-C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}d_{i,0}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}})}(t)\,d_{k,2}^{\dagger}\\
&-C_{\mathrm{L03}}^{(-)}C_{\mathrm{R21}}^{(-)}d_{i,0}^{\dagger}d_{j,1}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{k,2}^{\dagger}-C_{\mathrm{R03}}^{(-)}C_{\mathrm{R21}}^{(-)}d_{i,0}^{\dagger}d_{j,1}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{k,2}^{\dagger}\\
&-C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}d_{i,0}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{k,2}^{\dagger}-C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}d_{i,0}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-1)}(t)\,d_{k,2}^{\dagger}\\
&-C_{\mathrm{L03}}^{(-)}C_{\mathrm{L21}}^{(+)}d_{i,0}^{\dagger}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{k,2}-C_{\mathrm{R03}}^{(-)}C_{\mathrm{L21}}^{(+)}d_{i,0}^{\dagger}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{k,2}\\
&-C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(+)}d_{i,0}d_{j,1}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{k,2}-C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(+)}d_{i,0}d_{j,1}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}})}(t)\,d_{k,2}\\
&-C_{\mathrm{L03}}^{(-)}C_{\mathrm{R21}}^{(+)}d_{i,0}^{\dagger}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{k,2}-C_{\mathrm{R03}}^{(-)}C_{\mathrm{R21}}^{(+)}d_{i,0}^{\dagger}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{k,2}\\
&-C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(+)}d_{i,0}d_{j,1}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{k,2}-C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(+)}d_{i,0}d_{j,1}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+1)}(t)\,d_{k,2}\Big]\\
&+\mathrm{H.c.},
\end{aligned}
\tag{G.14}
$$

$$
\begin{aligned}
&\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{05,\mathrm{con}}\Big|_{03}\\
=&\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\times\Big[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L21}}^{(-)}d_{j,1}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-2,n_{\mathrm{R}})}(t)\,d_{k,2}^{\dagger}d_{i,0}^{\dagger}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R21}}^{(-)}d_{j,1}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}-1)}(t)\,d_{k,2}^{\dagger}d_{i,0}^{\dagger}
\end{aligned}
$$

$$
\begin{aligned}
&+C_{\mathrm{L03}}^{(-)}C_{\mathrm{L21}}^{(+)}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\,d_{k,2}d_{i,0}^{\dagger}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R21}}^{(+)}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}+1)}(t)\,d_{k,2}d_{i,0}^{\dagger}\\
&+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L21}}^{(-)}d_{j,1}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}-1)}(t)\,d_{k,2}^{\dagger}d_{i,0}^{\dagger}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R21}}^{(-)}d_{j,1}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-2)}(t)\,d_{k,2}^{\dagger}d_{i,0}^{\dagger}\\
&+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L21}}^{(+)}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}-1)}(t)\,d_{k,2}d_{i,0}^{\dagger}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R21}}^{(+)}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\,d_{k,2}d_{i,0}^{\dagger}\\
&+C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\,d_{k,2}^{\dagger}d_{i,0}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}-1)}(t)\,d_{k,2}^{\dagger}d_{i,0}\\
&+C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(+)}d_{j,1}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+2,n_{\mathrm{R}})}(t)\,d_{k,2}d_{i,0}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(+)}d_{j,1}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}+1)}(t)\,d_{k,2}d_{i,0}\\
&+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}+1)}(t)\,d_{k,2}^{\dagger}d_{i,0}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\,d_{k,2}^{\dagger}d_{i,0}\\
&\left.+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(+)}d_{j,1}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}+1)}(t)\,d_{k,2}d_{i,0}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(+)}d_{j,1}^{\dagger}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+2)}(t)\,d_{k,2}d_{i,0}\right]\\
&+\mathrm{H.c.},
\end{aligned}
\tag{G.15}
$$

$$
\begin{aligned}
&\quad \mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\Big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{05,\mathrm{con}}\Big|_{04}\\
&=\sum_{ijkl}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\\
&\quad\times\left[-C_{\mathrm{L03}}^{(-)}C_{\mathrm{L21}}^{(-)}d_{l,3}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-2,n_{\mathrm{R}})}(t)\,d_{k,2}^{\dagger}d_{i,0}^{\dagger}-C_{\mathrm{L03}}^{(-)}C_{\mathrm{R21}}^{(-)}d_{l,3}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}-1)}(t)\,d_{k,2}^{\dagger}d_{i,0}^{\dagger}\right.\\
&\quad-C_{\mathrm{L03}}^{(-)}C_{\mathrm{L21}}^{(+)}d_{l,3}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\,d_{k,2}d_{i,0}^{\dagger}-C_{\mathrm{L03}}^{(-)}C_{\mathrm{R21}}^{(+)}d_{l,3}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}+1)}(t)\,d_{k,2}d_{i,0}^{\dagger}\\
&\quad-C_{\mathrm{R03}}^{(-)}C_{\mathrm{L21}}^{(-)}d_{l,3}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}-1)}(t)\,d_{k,2}^{\dagger}d_{i,0}^{\dagger}-C_{\mathrm{R03}}^{(-)}C_{\mathrm{R21}}^{(-)}d_{l,3}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}-2)}(t)\,d_{k,2}^{\dagger}d_{i,0}^{\dagger}\\
&\quad-C_{\mathrm{R03}}^{(-)}C_{\mathrm{L21}}^{(+)}d_{l,3}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}-1)}(t)\,d_{k,2}d_{i,0}^{\dagger}-C_{\mathrm{R03}}^{(-)}C_{\mathrm{R21}}^{(+)}d_{l,3}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\,d_{k,2}d_{i,0}^{\dagger}\\
&\quad-C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}d_{l,3}^{\dagger}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\,d_{k,2}^{\dagger}d_{i,0}-C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}d_{l,3}^{\dagger}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}-1)}(t)\,d_{k,2}^{\dagger}d_{i,0}\\
&\quad-C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(+)}d_{l,3}^{\dagger}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+2,n_{\mathrm{R}})}(t)\,d_{k,2}d_{i,0}-C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(+)}d_{l,3}^{\dagger}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}+1)}(t)\,d_{k,2}d_{i,0}\\
&\quad-C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}d_{l,3}^{\dagger}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}-1,n_{\mathrm{R}}+1)}(t)\,d_{k,2}^{\dagger}d_{i,0}-C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}d_{l,3}^{\dagger}d_{j,1}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}})}(t)\,d_{k,2}^{\dagger}d_{i,0}\\
&\quad\left.-C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(+)}d_{l,3}^{\dagger}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}}+1,n_{\mathrm{R}}+1)}(t)\,d_{k,2}d_{i,0}-C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(+)}d_{l,3}^{\dagger}d_{j,1}^{\dagger}\rho_{\mathrm{QS}}^{(n_{\mathrm{L}},n_{\mathrm{R}}+2)}(t)\,d_{k,2}d_{i,0}\right]\\
&\quad+\mathrm{H.c.}.
\end{aligned}
\tag{G.16}
$$

# 附录 H　顺序隧穿极限下量子点系统的条件性约化密度矩阵元

在本附录中, 给出在顺序隧穿极限下, 第 5 章中单量子点、串联耦合双量子点以及 T 型双量子点的密度矩阵运动方程.

对于单量子点, 其密度矩阵的矩阵元 $\dot{\rho}_{\mathrm{dot},1,\uparrow\uparrow}^{(n)}(t)$、$\dot{\rho}_{\mathrm{dot},1,\downarrow\downarrow}^{(n)}(t)$ 以及 $\dot{\rho}_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}^{(n)}(t)$ 的运动方程分别为

$$
\dot{\rho}_{\mathrm{dot},1,\uparrow\uparrow}^{(n)}\Big|_{01}=\mathrm{i}\frac{\Gamma_{\mathrm{L}\uparrow}}{2\pi}\left[I_{2,\mathrm{L}+}(\varepsilon_{\uparrow})+I_{1,\mathrm{L}+}(\varepsilon_{\uparrow})\right]\rho_{\mathrm{dot},1,00}^{(n)}
$$

$$+\mathrm{i}\frac{\Gamma_{\mathrm{R}\uparrow}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_{\uparrow}\right)+I_{1,\mathrm{R}+}\left(\varepsilon_{\uparrow}\right)\right]\rho_{\mathrm{dot},1,00}^{(n+1)}, \tag{H.1-1}$$

$$\begin{aligned}\left.\dot{\rho}_{\mathrm{dot},1,\uparrow\uparrow}^{(n)}\right|_{02}=&-\mathrm{i}\frac{\Gamma_{\mathrm{L}\uparrow}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{\uparrow}\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{\uparrow}\right)\right]\rho_{\mathrm{dot},1,\uparrow\uparrow}^{(n)}\\&-\mathrm{i}\frac{\Gamma_{\mathrm{R}\uparrow}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{\uparrow}\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{\uparrow}\right)\right]\rho_{\mathrm{dot},1,\uparrow\uparrow}^{(n)}\\&-\mathrm{i}\frac{\Gamma_{\mathrm{L}\downarrow}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow}\right)+I_{1,\mathrm{L}+}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow}\right)\right]\rho_{\mathrm{dot},1,\uparrow\uparrow}^{(n)}\\&-\mathrm{i}\frac{\Gamma_{\mathrm{R}\downarrow}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow}\right)+I_{1,\mathrm{R}+}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow}\right)\right]\rho_{\mathrm{dot},1,\uparrow\uparrow}^{(n)},\end{aligned} \tag{H.1-2}$$

$$\begin{aligned}\left.\dot{\rho}_{\mathrm{dot},1,\uparrow\uparrow}^{(n)}\right|_{03}=&\,\mathrm{i}\frac{\Gamma_{\mathrm{L}\downarrow}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow}\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow}\right)\right]\rho_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}^{(n)}\\&+\mathrm{i}\frac{\Gamma_{\mathrm{R}\downarrow}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow}\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow}\right)\right]\rho_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}^{(n-1)}.\end{aligned} \tag{H.1-3}$$

$$\begin{aligned}\left.\dot{\rho}_{\mathrm{dot},1,\downarrow\downarrow}^{(n)}\right|_{01}=&\,\mathrm{i}\frac{\Gamma_{\mathrm{L}\downarrow}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_{\downarrow}\right)+I_{1,\mathrm{L}+}\left(\varepsilon_{\downarrow}\right)\right]\rho_{\mathrm{dot},1,00}^{(n)}\\&+\mathrm{i}\frac{\Gamma_{\mathrm{R}\downarrow}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_{\downarrow}\right)+I_{1,\mathrm{R}+}\left(\varepsilon_{\downarrow}\right)\right]\rho_{\mathrm{dot},1,00}^{(n+1)},\end{aligned} \tag{H.2-1}$$

$$\begin{aligned}\left.\dot{\rho}_{\mathrm{dot},1,\downarrow\downarrow}^{(n)}\right|_{02}=&-\mathrm{i}\frac{\Gamma_{\mathrm{L}\downarrow}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{\downarrow}\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{\downarrow}\right)\right]\rho_{\mathrm{dot},1,\downarrow\downarrow}^{(n)}\\&-\mathrm{i}\frac{\Gamma_{\mathrm{R}\downarrow}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{\downarrow}\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{\downarrow}\right)\right]\rho_{\mathrm{dot},1,\downarrow\downarrow}^{(n)}\\&-\mathrm{i}\frac{\Gamma_{\mathrm{L}\uparrow}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow}\right)+I_{1,\mathrm{L}+}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow}\right)\right]\rho_{\mathrm{dot},1,\downarrow\downarrow}^{(n)}\\&-\mathrm{i}\frac{\Gamma_{\mathrm{R}\uparrow}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow}\right)+I_{1,\mathrm{R}+}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow}\right)\right]\rho_{\mathrm{dot},1,\downarrow\downarrow}^{(n)},\end{aligned} \tag{H.2-2}$$

$$\begin{aligned}\left.\dot{\rho}_{\mathrm{dot},1,\downarrow\downarrow}^{(n)}\right|_{03}=&\,\mathrm{i}\frac{\Gamma_{\mathrm{L}\uparrow}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow}\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow}\right)\right]\rho_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}^{(n)}\\&+\mathrm{i}\frac{\Gamma_{\mathrm{R}\uparrow}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow}\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow}\right)\right]\rho_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}^{(n-1)}.\end{aligned} \tag{H.2-3}$$

$$\begin{aligned}\left.\dot{\rho}_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}^{(n)}\right|_{01}=&\,\mathrm{i}\frac{\Gamma_{\mathrm{L}\downarrow}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow}\right)+I_{1,\mathrm{L}+}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow}\right)\right]\rho_{\mathrm{dot},1,\uparrow\uparrow}^{(n)}\\&+\mathrm{i}\frac{\Gamma_{\mathrm{R}\downarrow}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow}\right)+I_{1,\mathrm{R}+}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow}\right)\right]\rho_{\mathrm{dot},1,\uparrow\uparrow}^{(n+1)},\end{aligned} \tag{H.3-1}$$

$$\left.\dot{\rho}_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}^{(n)}\right|_{02}=\mathrm{i}\frac{\Gamma_{\mathrm{L}\uparrow}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow}\right)+I_{1,\mathrm{L}+}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow}\right)\right]\rho_{\mathrm{dot},1,\downarrow\downarrow}^{(n)}$$

$$+\,\mathrm{i}\frac{\Gamma_{\mathrm{R}\uparrow}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow}\right)+I_{1,\mathrm{R}+}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow}\right)\right]\rho^{(n+1)}_{\mathrm{dot},1,\downarrow\downarrow},\tag{H.3-2}$$

$$\begin{aligned}\dot{\rho}^{(n)}_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}\Big|_{03}=&-\mathrm{i}\frac{\Gamma_{\mathrm{L}\uparrow}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow}\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow}\right)\right]\rho^{(n)}_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}\\&-\mathrm{i}\frac{\Gamma_{\mathrm{R}\uparrow}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow}\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\downarrow}\right)\right]\rho^{(n)}_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}\\&-\mathrm{i}\frac{\Gamma_{\mathrm{L}\downarrow}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow}\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow}\right)\right]\rho^{(n)}_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}\\&-\mathrm{i}\frac{\Gamma_{\mathrm{R}\downarrow}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow}\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{\uparrow,\downarrow}-\varepsilon_{\uparrow}\right)\right]\rho^{(n)}_{\mathrm{dot},1,\uparrow\downarrow,\uparrow\downarrow}.\end{aligned}\tag{H.3-3}$$

对于串联耦合双量子点，其密度矩阵的矩阵元 $\dot{\rho}^{(n)}_{\mathrm{dot},2,++}(t)$、$\dot{\rho}^{(n)}_{\mathrm{dot},2,+-}(t)$、$\dot{\rho}^{(n)}_{\mathrm{dot},2,-+}(t)$、$\dot{\rho}^{(n)}_{\mathrm{dot},2,--}(t)$ 以及 $\dot{\rho}^{(n)}_{\mathrm{dot},2,11,11}(t)$ 的运动方程分别为

$$\begin{aligned}\dot{\rho}^{(n)}_{\mathrm{dot},2,++}\Big|_{01}=&\frac{\mathrm{i}a_{+}a_{+}\Gamma_{\mathrm{L}}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_{+}\right)+I_{1,\mathrm{L}+}\left(\varepsilon_{+}\right)\right]\rho^{(n)}_{\mathrm{dot},2,00}\\&+\frac{\mathrm{i}b_{+}b_{+}\Gamma_{\mathrm{R}}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_{+}\right)+I_{1,\mathrm{R}+}\left(\varepsilon_{+}\right)\right]\rho^{(n+1)}_{\mathrm{dot},2,00},\end{aligned}\tag{H.4-1}$$

$$\begin{aligned}\dot{\rho}^{(n)}_{\mathrm{dot},2,++}\Big|_{02}=&-\frac{\mathrm{i}a_{+}a_{+}\Gamma_{\mathrm{L}}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{+}\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{+}\right)\right]\rho^{(n)}_{\mathrm{dot},2,++}\\&-\frac{\mathrm{i}b_{+}b_{+}\Gamma_{\mathrm{R}}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{+}\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{+}\right)\right]\rho^{(n)}_{\mathrm{dot},2,++}\\&-\mathrm{i}\frac{b_{+}b_{+}\Gamma_{\mathrm{L}}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)+I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)\right]\rho^{(n)}_{\mathrm{dot},2,++}\\&-\mathrm{i}\frac{a_{+}a_{+}\Gamma_{\mathrm{R}}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)+I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)\right]\rho^{(n)}_{\mathrm{dot},2,++},\end{aligned}\tag{H.4-2}$$

$$\begin{aligned}\dot{\rho}^{(n)}_{\mathrm{dot},2,++}\Big|_{03}=&-\frac{\mathrm{i}}{2\pi}\left[b_{+}b_{-}\Gamma_{\mathrm{L}}I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)+a_{+}a_{-}\Gamma_{\mathrm{R}}I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)\right]\rho^{(n)}_{\mathrm{dot},2,+-}\\&-\frac{\mathrm{i}}{2\pi}\left[a_{+}a_{-}\Gamma_{\mathrm{L}}I_{1,\mathrm{L}-}\left(\varepsilon_{-}\right)+b_{+}b_{-}\Gamma_{\mathrm{R}}I_{1,\mathrm{R}-}\left(\varepsilon_{-}\right)\right]\rho^{(n)}_{\mathrm{dot},2,+-},\end{aligned}\tag{H.4-3}$$

$$\begin{aligned}\dot{\rho}^{(n)}_{\mathrm{dot},2,++}\Big|_{04}=&-\frac{\mathrm{i}}{2\pi}\left[a_{+}a_{-}\Gamma_{\mathrm{L}}I_{2,\mathrm{L}-}\left(\varepsilon_{-}\right)+b_{+}b_{-}\Gamma_{R}I_{2,\mathrm{R}-}\left(\varepsilon_{-}\right)\right]\rho^{(n)}_{\mathrm{dot},2,-+}\\&-\frac{\mathrm{i}}{2\pi}\left[b_{+}b_{-}\Gamma_{\mathrm{L}}I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)+a_{+}a_{-}\Gamma_{\mathrm{R}}I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)\right]\rho^{(n)}_{\mathrm{dot},2,-+},\end{aligned}\tag{H.4-4}$$

$$\begin{aligned}\dot{\rho}^{(n)}_{\mathrm{dot},2,++}\Big|_{05}=&\,\mathrm{i}\frac{b_{+}b_{+}\Gamma_{\mathrm{L}}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)\right]\rho^{(n)}_{\mathrm{dot},2,11,11}\\&+\mathrm{i}\frac{a_{+}a_{+}\Gamma_{\mathrm{R}}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)\right]\rho^{(n-1)}_{\mathrm{dot},2,11,11}.\end{aligned}\tag{H.4-5}$$

$$\dot{\rho}^{(n)}_{\mathrm{dot},2,+-}\Big|_{01} = \frac{\mathrm{i}a_+a_-\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_-\right)+I_{1,\mathrm{L}+}\left(\varepsilon_+\right)\right]\rho^{(n)}_{\mathrm{dot},2,00} + \frac{\mathrm{i}b_+b_-\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_-\right)+I_{1,\mathrm{R}+}\left(\varepsilon_+\right)\right]\rho^{(n+1)}_{\mathrm{dot},2,00}, \tag{H.5-1}$$

$$\begin{aligned}\dot{\rho}^{(n)}_{\mathrm{dot},2,+-}\Big|_{02} =& -\frac{\mathrm{i}}{2\pi}\left[b_+b_-\Gamma_\mathrm{L}I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right.\\ &\left.+a_+a_-\Gamma_\mathrm{R}I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho^{(n)}_{\mathrm{dot},2,++}\\ &-\frac{\mathrm{i}}{2\pi}\left[a_+a_-\Gamma_\mathrm{L}I_{1,\mathrm{L}-}\left(\varepsilon_+\right)+b_+b_-\Gamma_\mathrm{R}I_{1,\mathrm{R}-}\left(\varepsilon_+\right)\right]\rho^{(n)}_{\mathrm{dot},2,++},\end{aligned} \tag{H.5-2}$$

$$\begin{aligned}\dot{\rho}^{(n)}_{\mathrm{dot},2,+-}\Big|_{03} =& -\mathrm{i}\left(\varepsilon_+-\varepsilon_-\right)\rho^{(n)}_{\mathrm{dot},2,+-}\\ &-\frac{\mathrm{i}\Gamma_\mathrm{L}}{2\pi}\left[b_-b_-I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)+b_+b_+I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho^{(n)}_{\mathrm{dot},2,+-}\\ &-\frac{\mathrm{i}\Gamma_\mathrm{R}}{2\pi}\left[a_-a_-I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)+a_+a_+I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho^{(n)}_{\mathrm{dot},2,+-}\\ &-\frac{\mathrm{i}\Gamma_\mathrm{L}}{2\pi}\left[a_+a_+I_{2,\mathrm{L}-}\left(\varepsilon_+\right)+a_-a_-I_{1,\mathrm{L}-}\left(\varepsilon_-\right)\right]\rho^{(n)}_{\mathrm{dot},2,+-}\\ &-\frac{\mathrm{i}\Gamma_\mathrm{R}}{2\pi}\left[b_+b_+I_{2,\mathrm{R}-}\left(\varepsilon_+\right)+b_-b_-I_{1,\mathrm{R}-}\left(\varepsilon_-\right)\right]\rho^{(n)}_{\mathrm{dot},2,+-},\end{aligned} \tag{H.5-3}$$

$$\begin{aligned}&\dot{\rho}^{(n)}_{\mathrm{dot},2,+-}\Big|_{04}\\ =& -\frac{\mathrm{i}}{2\pi}\left[a_+a_-\Gamma_\mathrm{L}I_{2,\mathrm{L}-}\left(\varepsilon_-\right)+b_+b_-\Gamma_RI_{2,\mathrm{R}-}\left(\varepsilon_-\right)\right]\rho^{(n)}_{\mathrm{dot},2,--}\\ &-\frac{\mathrm{i}}{2\pi}\left[b_+b_-\Gamma_\mathrm{L}I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right.\\ &\left.+a_+a_-\Gamma_\mathrm{R}I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho^{(n)}_{\mathrm{dot},2,--},\end{aligned} \tag{H.5-4}$$

$$\begin{aligned}&\dot{\rho}^{(n)}_{\mathrm{dot},2,+-}\Big|_{05}\\ =& \frac{\mathrm{i}b_+b_-\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_+\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho^{(n)}_{\mathrm{dot},2,11,11}\\ &+\frac{\mathrm{i}a_+a_-\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_+\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho^{(n-1)}_{\mathrm{dot},2,11,11}.\end{aligned} \tag{H.5-5}$$

$$\dot{\rho}^{(n)}_{\mathrm{dot},2,-+}\Big|_{01} = \frac{\mathrm{i}a_+a_-\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_+\right)+I_{1,\mathrm{L}+}\left(\varepsilon_-\right)\right]\rho^{(n)}_{\mathrm{dot},2,00} + \frac{\mathrm{i}b_+b_-\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_+\right)+I_{1,\mathrm{R}+}\left(\varepsilon_-\right)\right]\rho^{(n+1)}_{\mathrm{dot},2,00}, \tag{H.6-1}$$

$$\dot{\rho}^{(n)}_{\mathrm{dot},2,-+}\Big|_{02} = -\frac{\mathrm{i}}{2\pi}\left[b_+b_-\Gamma_\mathrm{L}I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)+a_+a_-\Gamma_\mathrm{R}I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho^{(n)}_{\mathrm{dot},2,++}$$

$$-\frac{\mathrm{i}}{2\pi}\left[a_{+}a_{-}\Gamma_{\mathrm{L}}I_{2,\mathrm{L}-}\left(\varepsilon_{+}\right)+b_{+}b_{-}\Gamma_{\mathrm{R}}I_{2,\mathrm{R}-}\left(\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},2,++}^{(n)}, \tag{H.6-2}$$

$$\begin{aligned}\left.\dot{\rho}_{\mathrm{dot},2,-+}^{(n)}\right|_{03}=&-\mathrm{i}\left(\varepsilon_{-}-\varepsilon_{+}\right)\rho_{\mathrm{dot},2,-+}^{(n)}\\&-\frac{\mathrm{i}\Gamma_{\mathrm{L}}}{2\pi}\left[b_{+}b_{+}I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)+b_{-}b_{-}I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)\right]\rho_{\mathrm{dot},2,-+}^{(n)}\\&-\frac{\mathrm{i}\Gamma_{\mathrm{R}}}{2\pi}\left[a_{+}a_{+}I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)+a_{-}a_{-}I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)\right]\rho_{\mathrm{dot},2,-+}^{(n)}\\&-\frac{\mathrm{i}\Gamma_{\mathrm{L}}}{2\pi}\left[a_{-}a_{-}I_{2,\mathrm{L}-}\left(\varepsilon_{-}\right)+a_{+}a_{+}I_{1,\mathrm{L}-}\left(\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},2,-+}^{(n)}\\&-\frac{\mathrm{i}\Gamma_{\mathrm{R}}}{2\pi}\left[b_{-}b_{-}I_{2,\mathrm{R}-}\left(\varepsilon_{-}\right)+b_{+}b_{+}I_{1,\mathrm{R}-}\left(\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},2,-+}^{(n)},\end{aligned} \tag{H.6-3}$$

$$\begin{aligned}\left.\dot{\rho}_{\mathrm{dot},2,-+}^{(n)}\right|_{04}=&-\frac{\mathrm{i}}{2\pi}\left[b_{+}b_{-}\Gamma_{\mathrm{L}}I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)+a_{+}a_{-}\Gamma_{\mathrm{R}}I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)\right]\rho_{\mathrm{dot},2,--}^{(n)}\\&-\frac{\mathrm{i}}{2\pi}\left[a_{+}a_{-}\Gamma_{\mathrm{L}}I_{1,\mathrm{L}-}\left(\varepsilon_{-}\right)+b_{+}b_{-}\Gamma_{\mathrm{R}}I_{1,\mathrm{R}-}\left(\varepsilon_{-}\right)\right]\rho_{\mathrm{dot},2,--}^{(n)},\end{aligned} \tag{H.6-4}$$

$$\begin{aligned}\left.\dot{\rho}_{\mathrm{dot},2,-+}^{(n)}\right|_{05}=&\frac{\mathrm{i}b_{+}b_{-}\Gamma_{\mathrm{L}}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},2,11,11}^{(n)}\\&+\frac{\mathrm{i}a_{+}a_{-}\Gamma_{\mathrm{R}}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},2,11,11}^{(n-1)}.\end{aligned} \tag{H.6-5}$$

$$\begin{aligned}\left.\dot{\rho}_{\mathrm{dot},2,--}^{(n)}\right|_{01}=&\frac{\mathrm{i}a_{-}a_{-}\Gamma_{\mathrm{L}}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_{-}\right)+I_{1,\mathrm{L}+}\left(\varepsilon_{-}\right)\right]\rho_{\mathrm{dot},2,00}^{(n)}\\&+\frac{\mathrm{i}b_{-}b_{-}\Gamma_{\mathrm{R}}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_{-}\right)+I_{1,\mathrm{R}+}\left(\varepsilon_{-}\right)\right]\rho_{\mathrm{dot},2,00}^{(n+1)},\end{aligned} \tag{H.7-1}$$

$$\begin{aligned}&\left.\dot{\rho}_{\mathrm{dot},2,--}^{(n)}\right|_{02}\\=&-\frac{\mathrm{i}}{2\pi}\left[a_{+}a_{-}\Gamma_{\mathrm{L}}I_{2,\mathrm{L}-}\left(\varepsilon_{+}\right)+b_{+}b_{-}\Gamma_{R}I_{2,\mathrm{R}-}\left(\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},2,+-}^{(n)}\\&-\frac{\mathrm{i}}{2\pi}\left[b_{+}b_{-}\Gamma_{\mathrm{L}}I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)+a_{+}a_{-}\Gamma_{\mathrm{R}}I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},2,+-}^{(n)},\end{aligned} \tag{H.7-2}$$

$$\begin{aligned}\left.\dot{\rho}_{\mathrm{dot},2,--}^{(n)}\right|_{03}=&-\frac{\mathrm{i}}{2\pi}\left[b_{+}b_{-}\Gamma_{\mathrm{L}}I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)+a_{+}a_{-}\Gamma_{\mathrm{R}}I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},2,-+}^{(n)}\\&-\frac{\mathrm{i}}{2\pi}\left[a_{+}a_{-}\Gamma_{\mathrm{L}}I_{1,\mathrm{L}-}\left(\varepsilon_{+}\right)+b_{+}b_{-}\Gamma_{\mathrm{R}}I_{1,\mathrm{R}-}\left(\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},2,-+}^{(n)},\end{aligned} \tag{H.7-3}$$

$$\left.\dot{\rho}_{\mathrm{dot},2,--}^{(n)}\right|_{04}=-\mathrm{i}\frac{b_{-}b_{-}\Gamma_{\mathrm{L}}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)+I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)\right]\rho_{\mathrm{dot},2,--}^{(n)}$$

$$- \mathrm{i}\frac{a_-a_-\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)+I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho^{(n)}_{\mathrm{dot},2,--}$$
$$- \frac{\mathrm{i}a_-a_-\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_-\right)+I_{1,\mathrm{L}-}\left(\varepsilon_-\right)\right]\rho^{(n)}_{\mathrm{dot},2,--}$$
$$- \frac{\mathrm{i}b_-b_-\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_-\right)+I_{1,\mathrm{R}-}\left(\varepsilon_-\right)\right]\rho^{(n)}_{\mathrm{dot},2,--}, \tag{H.7-4}$$

$$\begin{aligned}\dot{\rho}^{(n)}_{\mathrm{dot},2,--}\Big|_{05} =& \mathrm{i}\frac{b_-b_-\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_-\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho^{(n)}_{\mathrm{dot},2,11,11}\\ &+\mathrm{i}\frac{a_-a_-\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_-\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho^{(n-1)}_{\mathrm{dot},2,11,11}.\end{aligned} \tag{H.7-5}$$

$$\begin{aligned}\dot{\rho}^{(n)}_{\mathrm{dot},2,11,11}\Big|_{01} =& \mathrm{i}\frac{b_+b_+\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)+I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho^{(n)}_{\mathrm{dot},2,++}\\ &+\mathrm{i}\frac{a_+a_+\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)+I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho^{(n+1)}_{\mathrm{dot},2,++},\end{aligned} \tag{H.8-1}$$

$$\begin{aligned}\dot{\rho}^{(n)}_{\mathrm{dot},2,11,11}\Big|_{02} =& \frac{\mathrm{i}b_+b_-\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)+I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho^{(n)}_{\mathrm{dot},2,+-}\\ &+\frac{\mathrm{i}a_+a_-\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)+I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho^{(n+1)}_{\mathrm{dot},2,+-},\end{aligned} \tag{H.8-2}$$

$$\begin{aligned}\dot{\rho}^{(n)}_{\mathrm{dot},2,11,11}\Big|_{03} =& \frac{\mathrm{i}b_+b_-\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)+I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho^{(n)}_{\mathrm{dot},2,-+}\\ &+\frac{\mathrm{i}a_+a_-\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)+I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho^{(n+1)}_{\mathrm{dot},2,-+},\end{aligned} \tag{H.8-3}$$

$$\begin{aligned}\dot{\rho}^{(n)}_{\mathrm{dot},2,11,11}\Big|_{04} =& \mathrm{i}\frac{b_-b_-\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)+I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho^{(n)}_{\mathrm{dot},2,--}\\ &+\mathrm{i}\frac{a_-a_-\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)+I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho^{(n+1)}_{\mathrm{dot},2,--},\end{aligned} \tag{H.8-4}$$

$$\begin{aligned}\dot{\rho}^{(n)}_{\mathrm{dot},2,11,11}\Big|_{05} =& -\mathrm{i}\frac{b_+b_+\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_+\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho^{(n)}_{\mathrm{dot},2,11,11}\\ &-\mathrm{i}\frac{b_-b_-\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_-\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho^{(n)}_{\mathrm{dot},2,11,11}\\ &-\mathrm{i}\frac{a_+a_+\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_+\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho^{(n)}_{\mathrm{dot},2,11,11}\\ &-\mathrm{i}\frac{a_-a_-\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_-\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho^{(n)}_{\mathrm{dot},2,11,11}.\end{aligned} \tag{H.8-5}$$

对于 T 型双量子点，其密度矩阵的矩阵元 $\dot{\rho}^{(n)}_{\mathrm{dot},3,++}(t)$、$\dot{\rho}^{(n)}_{\mathrm{dot},3,+-}(t)$、$\dot{\rho}^{(n)}_{\mathrm{dot},3,-+}(t)$、$\dot{\rho}^{(n)}_{\mathrm{dot},3,--}(t)$ 以及 $\dot{\rho}^{(n)}_{\mathrm{dot},3,11,11}(t)$ 的运动方程分别为

$$\dot{\rho}^{(n)}_{\mathrm{dot},3,++}\Big|_{01} = \frac{\mathrm{i}a_+a_+\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_+\right)+I_{1,\mathrm{L}+}\left(\varepsilon_+\right)\right]\rho^{(n)}_{\mathrm{dot},3,00}$$

$$+\frac{\mathrm{i}a_+a_+\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_+\right)+I_{1,\mathrm{R}+}\left(\varepsilon_+\right)\right]\rho_{\mathrm{dot},3,00}^{(n+1)},\tag{H.9-1}$$

$$\begin{aligned}\dot{\rho}_{\mathrm{dot},3,++}^{(n)}\Big|_{02}=&-\mathrm{i}\frac{b_+b_+\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)+I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho_{\mathrm{dot},3,++}^{(n)}\\&-\mathrm{i}\frac{b_+b_+\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)+I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho_{\mathrm{dot},3,++}^{(n)}\\&-\frac{\mathrm{i}a_+a_+\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_+\right)+I_{1,\mathrm{L}-}\left(\varepsilon_+\right)\right]\rho_{\mathrm{dot},3,++}^{(n)}\\&-\frac{\mathrm{i}a_+a_+\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_+\right)+I_{1,\mathrm{R}-}\left(\varepsilon_+\right)\right]\rho_{\mathrm{dot},3,++}^{(n)},\end{aligned}\tag{H.9-2}$$

$$\begin{aligned}\dot{\rho}_{\mathrm{dot},3,++}^{(n)}\Big|_{03}=&-\frac{\mathrm{i}b_+b_-}{2\pi}\left[\Gamma_\mathrm{L}I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)+\Gamma_\mathrm{R}I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho_{\mathrm{dot},3,+-}^{(n)}\\&-\frac{\mathrm{i}a_+a_-}{2\pi}\left[\Gamma_\mathrm{L}I_{1,\mathrm{L}-}\left(\varepsilon_-\right)+\Gamma_\mathrm{R}I_{1,\mathrm{R}-}\left(\varepsilon_-\right)\right]\rho_{\mathrm{dot},3,+-}^{(n)},\end{aligned}\tag{H.9-3}$$

$$\begin{aligned}\dot{\rho}_{\mathrm{dot},3,++}^{(n)}\Big|_{04}=&-\frac{\mathrm{i}a_+a_-}{2\pi}\left[\Gamma_\mathrm{L}I_{2,\mathrm{L}-}\left(\varepsilon_-\right)+\Gamma_\mathrm{R}I_{2,\mathrm{R}-}\left(\varepsilon_-\right)\right]\rho_{\mathrm{dot},3,-+}^{(n)}\\&-\frac{\mathrm{i}b_+b_-}{2\pi}\left[\Gamma_\mathrm{L}I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)+\Gamma_\mathrm{R}I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho_{\mathrm{dot},3,-+}^{(n)},\end{aligned}\tag{H.9-4}$$

$$\begin{aligned}\dot{\rho}_{\mathrm{dot},3,++}^{(n)}\Big|_{05}=&\,\mathrm{i}\frac{b_+b_+\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_+\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho_{\mathrm{dot},3,11,11}^{(n)}\\&+\mathrm{i}\frac{b_+b_+\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_+\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho_{\mathrm{dot},3,11,11}^{(n-1)}.\end{aligned}\tag{H.9-5}$$

$$\begin{aligned}\dot{\rho}_{\mathrm{dot},3,+-}^{(n)}\Big|_{01}=&\,\frac{\mathrm{i}a_+a_-\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_-\right)+I_{1,\mathrm{L}+}\left(\varepsilon_+\right)\right]\rho_{\mathrm{dot},3,00}^{(n)}\\&+\frac{\mathrm{i}a_+a_-\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_-\right)+I_{1,\mathrm{R}+}\left(\varepsilon_+\right)\right]\rho_{\mathrm{dot},3,00}^{(n+1)},\end{aligned}\tag{H.10-1}$$

$$\begin{aligned}\dot{\rho}_{\mathrm{dot},3,+-}^{(n)}\Big|_{02}=&-\frac{\mathrm{i}b_+b_-}{2\pi}\left[\Gamma_\mathrm{L}I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)+\Gamma_\mathrm{R}I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho_{\mathrm{dot},3,++}^{(n)}\\&-\frac{\mathrm{i}a_+a_-}{2\pi}\left[\Gamma_\mathrm{L}I_{1,\mathrm{L}-}\left(\varepsilon_+\right)+\Gamma_\mathrm{R}I_{1,\mathrm{R}-}\left(\varepsilon_+\right)\right]\rho_{\mathrm{dot},3,++}^{(n)},\end{aligned}\tag{H.10-2}$$

$$\begin{aligned}\dot{\rho}_{\mathrm{dot},3,+-}^{(n)}\Big|_{03}=&-\mathrm{i}\left(\varepsilon_+-\varepsilon_-\right)\rho_{\mathrm{dot},3,+-}^{(n)}\\&-\frac{\mathrm{i}\Gamma_\mathrm{L}}{2\pi}\left[b_-b_-I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)+b_+b_+I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho_{\mathrm{dot},3,+-}^{(n)}\\&-\frac{\mathrm{i}\Gamma_\mathrm{R}}{2\pi}\left[b_-b_-I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)+b_+b_+I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho_{\mathrm{dot},3,+-}^{(n)}\\&-\frac{\mathrm{i}\Gamma_\mathrm{L}}{2\pi}\left[a_+a_+I_{2,\mathrm{L}-}\left(\varepsilon_+\right)+a_-a_-I_{1,\mathrm{L}-}\left(\varepsilon_-\right)\right]\rho_{\mathrm{dot},3,+-}^{(n)}\end{aligned}$$

$$-\frac{\mathrm{i}\Gamma_{\mathrm{R}}}{2\pi}\left[a_{+}a_{+}I_{2,\mathrm{R}-}\left(\varepsilon_{+}\right)+a_{-}a_{-}I_{1,\mathrm{R}-}\left(\varepsilon_{-}\right)\right]\rho_{\mathrm{dot},3,+-}^{(n)}, \tag{H.10-3}$$

$$\begin{aligned}\left.\dot{\rho}_{\mathrm{dot},3,+-}^{(n)}\right|_{04}=&-\frac{\mathrm{i}a_{+}a_{-}}{2\pi}\left[\Gamma_{\mathrm{L}}I_{2,\mathrm{L}-}\left(\varepsilon_{-}\right)+\Gamma_{\mathrm{R}}I_{2,\mathrm{R}-}\left(\varepsilon_{-}\right)\right]\rho_{\mathrm{dot},3,--}^{(n)}\\&-\frac{\mathrm{i}b_{+}b_{-}}{2\pi}\left[\Gamma_{\mathrm{L}}I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)+\Gamma_{\mathrm{R}}I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)\right]\rho_{\mathrm{dot},3,--}^{(n)},\end{aligned} \tag{H.10-4}$$

$$\begin{aligned}\left.\dot{\rho}_{\mathrm{dot},3,+-}^{(n)}\right|_{05}=&\frac{\mathrm{i}b_{+}b_{-}\Gamma_{\mathrm{L}}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)\right]\rho_{\mathrm{dot},3,11,11}^{(n)}\\&+\frac{\mathrm{i}b_{+}b_{-}\Gamma_{\mathrm{R}}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)\right]\rho_{\mathrm{dot},3,11,11}^{(n-1)}.\end{aligned} \tag{H.10-5}$$

$$\begin{aligned}\left.\dot{\rho}_{\mathrm{dot},3,-+}^{(n)}\right|_{01}=&\frac{\mathrm{i}a_{+}a_{-}\Gamma_{\mathrm{L}}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_{+}\right)+I_{1,\mathrm{L}+}\left(\varepsilon_{-}\right)\right]\rho_{\mathrm{dot},3,00}^{(n)}\\&+\frac{\mathrm{i}a_{+}a_{-}\Gamma_{\mathrm{R}}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_{+}\right)+I_{1,\mathrm{R}+}\left(\varepsilon_{-}\right)\right]\rho_{\mathrm{dot},3,00}^{(n+1)},\end{aligned} \tag{H.11-1}$$

$$\begin{aligned}\left.\dot{\rho}_{\mathrm{dot},3,-+}^{(n)}\right|_{02}=&-\frac{\mathrm{i}a_{+}a_{-}}{2\pi}\left[\Gamma_{\mathrm{L}}I_{2,\mathrm{L}-}\left(\varepsilon_{+}\right)+\Gamma_{\mathrm{R}}I_{2,\mathrm{R}-}\left(\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},3,++}^{(n)}\\&-\frac{\mathrm{i}b_{+}b_{-}}{2\pi}\left[\Gamma_{\mathrm{L}}I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)+\Gamma_{\mathrm{R}}I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},3,++}^{(n)},\end{aligned} \tag{H.11-2}$$

$$\begin{aligned}\left.\dot{\rho}_{\mathrm{dot},3,-+}^{(n)}\right|_{03}=&-\mathrm{i}\left(\varepsilon_{-}-\varepsilon_{+}\right)\rho_{\mathrm{dot},3,-+}^{(n)}\\&-\frac{\mathrm{i}\Gamma_{\mathrm{L}}}{2\pi}\left[b_{+}b_{+}I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)+b_{-}b_{-}I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)\right]\rho_{\mathrm{dot},3,-+}^{(n)}\\&-\frac{\mathrm{i}\Gamma_{\mathrm{R}}}{2\pi}\left[b_{+}b_{+}I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)+b_{-}b_{-}I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)\right]\rho_{\mathrm{dot},3,-+}^{(n)}\\&-\frac{\mathrm{i}\Gamma_{\mathrm{L}}}{2\pi}\left[a_{-}a_{-}I_{2,\mathrm{L}-}\left(\varepsilon_{-}\right)+a_{+}a_{+}I_{1,\mathrm{L}-}\left(\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},3,-+}^{(n)}\\&-\frac{\mathrm{i}\Gamma_{\mathrm{R}}}{2\pi}\left[a_{-}a_{-}I_{2,\mathrm{R}-}\left(\varepsilon_{-}\right)+a_{+}a_{+}I_{1,\mathrm{R}-}\left(\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},3,-+}^{(n)},\end{aligned} \tag{H.11-3}$$

$$\begin{aligned}\left.\dot{\rho}_{\mathrm{dot},3,-+}^{(n)}\right|_{04}=&-\frac{\mathrm{i}b_{+}b_{-}}{2\pi}\left[\Gamma_{\mathrm{L}}I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)+\Gamma_{\mathrm{R}}I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)\right]\rho_{\mathrm{dot},3,--}^{(n)}\\&-\frac{\mathrm{i}a_{+}a_{-}}{2\pi}\left[\Gamma_{\mathrm{L}}I_{1,\mathrm{L}-}\left(\varepsilon_{-}\right)+\Gamma_{\mathrm{R}}I_{1,\mathrm{R}-}\left(\varepsilon_{-}\right)\right]\rho_{\mathrm{dot},3,--}^{(n)},\end{aligned} \tag{H.11-4}$$

$$\begin{aligned}\left.\dot{\rho}_{\mathrm{dot},3,-+}^{(n)}\right|_{05}=&\frac{\mathrm{i}b_{+}b_{-}\Gamma_{\mathrm{L}}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},3,11,11}^{(n)}\\&+\frac{\mathrm{i}b_{+}b_{-}\Gamma_{\mathrm{R}}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_{-}\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_{+}\right)\right]\rho_{\mathrm{dot},3,11,11}^{(n-1)}.\end{aligned} \tag{H.11-5}$$

$$\dot{\rho}^{(n)}_{\text{dot},3,--}\Big|_{01} = \frac{\text{i}a_- a_- \Gamma_\text{L}}{2\pi}\left[I_{2,\text{L}+}\left(\varepsilon_-\right) + I_{1,\text{L}+}\left(\varepsilon_-\right)\right]\rho^{(n)}_{\text{dot},3,00} + \frac{\text{i}a_- a_- \Gamma_\text{R}}{2\pi}\left[I_{2,\text{R}+}\left(\varepsilon_-\right) + I_{1,\text{R}+}\left(\varepsilon_-\right)\right]\rho^{(n+1)}_{\text{dot},3,00}, \tag{H.12-1}$$

$$\dot{\rho}^{(n)}_{\text{dot},3,--}\Big|_{02} = -\frac{\text{i}a_+ a_-}{2\pi}\left[\Gamma_\text{L} I_{2,\text{L}-}\left(\varepsilon_+\right) + \Gamma_\text{R} I_{2,\text{R}-}\left(\varepsilon_+\right)\right]\rho^{(n)}_{\text{dot},3,+-} - \frac{\text{i}b_+ b_-}{2\pi}\left[\Gamma_\text{L} I_{1,\text{L}+}\left(\varepsilon_{1,1}-\varepsilon_+\right) + \Gamma_\text{R} I_{1,\text{R}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho^{(n)}_{\text{dot},3,+-}, \tag{H.12-2}$$

$$\dot{\rho}^{(n)}_{\text{dot},3,--}\Big|_{03} = -\frac{\text{i}b_+ b_-}{2\pi}\left[\Gamma_\text{L} I_{2,\text{L}+}\left(\varepsilon_{1,1}-\varepsilon_+\right) + \Gamma_\text{R} I_{2,\text{R}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho^{(n)}_{\text{dot},3,-+} - \frac{\text{i}a_+ a_-}{2\pi}\left[\Gamma_\text{L} I_{1,\text{L}-}\left(\varepsilon_+\right) + \Gamma_\text{R} I_{1,\text{R}-}\left(\varepsilon_+\right)\right]\rho^{(n)}_{\text{dot},3,-+}, \tag{H.12-3}$$

$$\begin{aligned}\dot{\rho}^{(n)}_{\text{dot},3,--}\Big|_{04} = &-\text{i}\frac{b_- b_- \Gamma_\text{L}}{2\pi}\left[I_{2,\text{L}+}\left(\varepsilon_{1,1}-\varepsilon_-\right) + I_{1,\text{L}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho^{(n)}_{\text{dot},3,--}\\ &- \text{i}\frac{b_- b_- \Gamma_\text{R}}{2\pi}\left[I_{2,\text{R}+}\left(\varepsilon_{1,1}-\varepsilon_-\right) + I_{1,\text{R}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho^{(n)}_{\text{dot},3,--}\\ &- \frac{\text{i}a_- a_- \Gamma_\text{L}}{2\pi}\left[I_{2,\text{L}-}\left(\varepsilon_-\right) + I_{1,\text{L}-}\left(\varepsilon_-\right)\right]\rho^{(n)}_{\text{dot},3,--}\\ &- \frac{\text{i}a_- a_- \Gamma_\text{R}}{2\pi}\left[I_{2,\text{R}-}\left(\varepsilon_-\right) + I_{1,\text{R}-}\left(\varepsilon_-\right)\right]\rho^{(n)}_{\text{dot},3,--},\end{aligned} \tag{H.12-4}$$

$$\dot{\rho}^{(n)}_{\text{dot},3,--}\Big|_{05} = \text{i}\frac{b_- b_- \Gamma_\text{L}}{2\pi}\left[I_{2,\text{L}-}\left(\varepsilon_{1,1}-\varepsilon_-\right) + I_{1,\text{L}-}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho^{(n)}_{\text{dot},3,11,11} + \text{i}\frac{b_- b_- \Gamma_\text{R}}{2\pi}\left[I_{2,\text{R}-}\left(\varepsilon_{1,1}-\varepsilon_-\right) + I_{1,\text{R}-}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho^{(n-1)}_{\text{dot},3,11,11}. \tag{H.12-5}$$

$$\dot{\rho}^{(n)}_{\text{dot},3,11,11}\Big|_{01} = \text{i}\frac{b_+ b_+ \Gamma_\text{L}}{2\pi}\left[I_{2,\text{L}+}\left(\varepsilon_{1,1}-\varepsilon_+\right) + I_{1,\text{L}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho^{(n)}_{\text{dot},3,++} + \text{i}\frac{b_+ b_+ \Gamma_\text{R}}{2\pi}\left[I_{2,\text{R}+}\left(\varepsilon_{1,1}-\varepsilon_+\right) + I_{1,\text{R}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho^{(n+1)}_{\text{dot},3,++}, \tag{H.13-1}$$

$$\begin{aligned}&\dot{\rho}^{(n)}_{\text{dot},3,11,11}\Big|_{02}\\ &= \frac{\text{i}b_+ b_-}{2\pi}\left[\Gamma_\text{L} I_{2,\text{L}+}\left(\varepsilon_{1,1}-\varepsilon_-\right) + \Gamma_\text{L} I_{1,\text{L}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho^{(n)}_{\text{dot},3,+-}\\ &+ \frac{\text{i}b_+ b_-}{2\pi}\left[\Gamma_\text{R} I_{2,\text{R}+}\left(\varepsilon_{1,1}-\varepsilon_-\right) + \Gamma_\text{R} I_{1,\text{R}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho^{(n+1)}_{\text{dot},3,+-},\end{aligned} \tag{H.13-2}$$

$$\begin{aligned}&\dot{\rho}^{(n)}_{\text{dot},3,11,11}\Big|_{03}\\ &= \frac{\text{i}b_+ b_-}{2\pi}\left[\Gamma_\text{L} I_{2,\text{L}+}\left(\varepsilon_{1,1}-\varepsilon_+\right) + \Gamma_\text{L} I_{1,\text{L}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho^{(n)}_{\text{dot},3,-+}\end{aligned}$$

$$+\frac{\mathrm{i}b_+b_-}{2\pi}\left[\Gamma_\mathrm{R}I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_+\right)+\Gamma_\mathrm{R}I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho_{\mathrm{dot},3,-+}^{(n+1)}, \tag{H.13-3}$$

$$\begin{aligned}&\dot{\rho}_{\mathrm{dot},3,11,11}^{(n)}\Big|_{04}\\ =&\,\mathrm{i}\frac{b_-b_-\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)+I_{1,\mathrm{L}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho_{\mathrm{dot},3,--}^{(n)}\\ &+\mathrm{i}\frac{b_-b_-\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)+I_{1,\mathrm{R}+}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho_{\mathrm{dot},3,--}^{(n+1)},\end{aligned} \tag{H.13-4}$$

$$\begin{aligned}&\dot{\rho}_{\mathrm{dot},3,11,11}^{(n)}\Big|_{05}\\ =&-\mathrm{i}\frac{b_+b_+\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_+\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho_{\mathrm{dot},3,11,11}^{(n)}\\ &-\mathrm{i}\frac{b_-b_-\Gamma_\mathrm{L}}{2\pi}\left[I_{2,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_-\right)+I_{1,\mathrm{L}-}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho_{\mathrm{dot},3,11,11}^{(n)}\\ &-\mathrm{i}\frac{b_+b_+\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_+\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_+\right)\right]\rho_{\mathrm{dot},3,11,11}^{(n)}\\ &-\mathrm{i}\frac{b_-b_-\Gamma_\mathrm{R}}{2\pi}\left[I_{2,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_-\right)+I_{1,\mathrm{R}-}\left(\varepsilon_{1,1}-\varepsilon_-\right)\right]\rho_{\mathrm{dot},3,11,11}^{(n)}.\end{aligned} \tag{H.13-5}$$

# 附录 I 共隧穿极限下 T 型双量子点的条件性约化密度矩阵元

在本附录中, 给出在 T 型双量子点中描述电子共隧穿过程的密度矩阵元 $\dot{\rho}_{\mathrm{S,co},00}^{(n)}(t)$ 的表示式. 对于 $\dot{\rho}_{\mathrm{S,co},00}^{(n)}(t)$ 的第一部分, 由式 (4.72)~式 (4.75) 可得

$$\begin{aligned}&\langle 0|\mathrm{e}^{-\mathrm{i}H_\mathrm{QS}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_\mathrm{QS}t}\big|_{01,\mathrm{con}}\Big|_{01}|0\rangle\\ =&\sum_{ijkl}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\Big[C_{02}^{(+)}C_{13}^{(-)}\langle 0|\,d_{i,0}d_{j,1}^{\dagger}d_{k,2}^{\dagger}d_{l,3}\rho_\mathrm{QS}^{(n)}(t)\,|0\rangle\\ &+C_{02}^{(+)}C_{13}^{(+)}\langle 0|\,d_{i,0}d_{j,1}d_{k,2}^{\dagger}d_{l,3}^{\dagger}\rho_\mathrm{QS}^{(n)}(t)\,|0\rangle\Big]+\mathrm{H.c.},\end{aligned} \tag{I.1}$$

$$\begin{aligned}&\langle 0|\mathrm{e}^{-\mathrm{i}H_\mathrm{QS}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_\mathrm{QS}t}\big|_{01,\mathrm{con}}\Big|_{02}|0\rangle\\ =&-\sum_{ijkl}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\Big[C_{02}^{(+)}C_{13}^{(-)}\langle 0|\,d_{i,0}d_{k,2}^{\dagger}d_{j,1}^{\dagger}d_{l,3}\rho_\mathrm{QS}^{(n)}(t)\,|0\rangle\\ &+C_{02}^{(+)}C_{13}^{(+)}\langle 0|\,d_{i,0}d_{k,2}^{\dagger}d_{j,1}d_{l,3}^{\dagger}\rho_\mathrm{QS}^{(n)}(t)\,|0\rangle\Big]+\mathrm{H.c.},\end{aligned} \tag{I.2}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{01,\mathrm{con}}\Big|_{03}|0\rangle$$

$$\begin{aligned}
&=\sum_{ijkl}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\Big[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L13}}^{(-)}\langle 0|\,d_{k,2}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n)}(t)\,d_{i,0}^{\dagger}\,|0\rangle\\
&+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R13}}^{(-)}\langle 0|\,d_{k,2}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n)}(t)\,d_{i,0}^{\dagger}\,|0\rangle\\
&+C_{\mathrm{L02}}^{(-)}C_{\mathrm{L13}}^{(+)}\langle 0|\,d_{k,2}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n)}(t)\,d_{i,0}^{\dagger}\,|0\rangle\\
&+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R13}}^{(+)}\langle 0|\,d_{k,2}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n)}(t)\,d_{i,0}^{\dagger}\,|0\rangle\\
&+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L13}}^{(-)}\langle 0|\,d_{k,2}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n-1)}(t)\,d_{i,0}^{\dagger}\,|0\rangle\\
&+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R13}}^{(-)}\langle 0|\,d_{k,2}d_{j,1}^{\dagger}d_{l,3}\rho_{\mathrm{QS}}^{(n-1)}(t)\,d_{i,0}^{\dagger}\,|0\rangle\\
&+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L13}}^{(+)}\langle 0|\,d_{k,2}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n-1)}(t)\,d_{i,0}^{\dagger}\,|0\rangle\\
&+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R13}}^{(+)}\langle 0|\,d_{k,2}d_{j,1}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n-1)}(t)\,d_{i,0}^{\dagger}\,|0\rangle\Big]+\mathrm{H.c.},
\end{aligned}\tag{I.3}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{01,\mathrm{con}}\Big|_{04}|0\rangle$$

$$\begin{aligned}
&=-\sum_{ijkl}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\Big[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L13}}^{(+)}\langle 0|\,d_{j,1}d_{k,2}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n)}(t)\,d_{i,0}^{\dagger}\\
&+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R13}}^{(+)}\langle 0|\,d_{j,1}d_{k,2}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n)}(t)\,d_{i,0}^{\dagger}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L13}}^{(+)}\langle 0|\,d_{j,1}d_{k,2}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n-1)}(t)\,d_{i,0}^{\dagger}\\
&+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R13}}^{(+)}\langle 0|\,d_{j,1}d_{k,2}d_{l,3}^{\dagger}\rho_{\mathrm{QS}}^{(n-1)}(t)\,d_{i,0}^{\dagger}\Big]+\mathrm{H.c.}.
\end{aligned}\tag{I.4}$$

将算符记号的式 (4.60)~式 (4.67) 代入式 (I.1)~式 (I.4) 可得

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{01,\mathrm{con}}\Big|_{01}|0\rangle$$

$$\begin{aligned}
&=\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\\
&\times\Big[C_{02}^{(+)}C_{13}^{(-)}\langle 0|\,d_1\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}(t-t_1)}d_1^{\dagger}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t_2-t_1)}d_1^{\dagger}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t_3-t_2)}d_1\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_3)}\rho_{\mathrm{QS}}^{(n)}(t)\,|0\rangle\\
&+C_{02}^{(+)}C_{13}^{(+)}\langle 0|\,d_1\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}(t-t_1)}d_1\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t_2-t_1)}d_1^{\dagger}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t_3-t_2)}d_1^{\dagger}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_3)}\rho_{\mathrm{QS}}^{(n)}(t)\,|0\rangle\Big]\\
&+\mathrm{H.c.},
\end{aligned}\tag{I.5}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{01,\mathrm{con}}\Big|_{02}|0\rangle$$

$$=-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3$$

$$\times \Big[ C_{02}^{(+)} C_{13}^{(-)} \langle 0 | d_1 e^{-iH_{QS}(t-t_2)} d_1^{\dagger} e^{iH_{QS}(t_1-t_2)} d_1^{\dagger} e^{iH_{QS}(t_3-t_1)} d_1 e^{iH_{QS}(t-t_3)} \rho_{QS}^{(n)}(t) |0\rangle$$
$$+ C_{02}^{(+)} C_{13}^{(+)} \langle 0 | d_1 e^{-iH_{QS}(t-t_2)} d_1^{\dagger} e^{iH_{QS}(t_1-t_2)} d_1 e^{iH_{QS}(t_3-t_1)} d_1^{\dagger} e^{iH_{QS}(t-t_3)} \rho_{QS}^{(n)}(t) |0\rangle \Big]$$
$$+ \text{H.c.}, \tag{I.6}$$

$$\langle 0 | e^{-iH_{QS}t} \rho_{QS,I}(t) \big|_{\text{fourth-order}} e^{iH_{QS}t} \big|_{01,\text{con}} \big|_{03} |0\rangle$$
$$= \int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \int_{-\infty}^{t_2} dt_3$$
$$\times \Big[ C_{L02}^{(-)} C_{L13}^{(-)} \langle 0 | e^{-iH_{QS}(t-t_2)} d_1 e^{iH_{QS}(t_1-t_2)} d_1^{\dagger} e^{iH_{QS}(t_3-t_1)} d_1 e^{iH_{QS}(t-t_3)} \rho_{QS}^{(n)}(t) d_1^{\dagger} |0\rangle$$
$$+ C_{L02}^{(-)} C_{R13}^{(-)} \langle 0 | e^{-iH_{QS}(t-t_2)} d_1 e^{iH_{QS}(t_1-t_2)} d_1^{\dagger} e^{iH_{QS}(t_3-t_1)} d_1 e^{iH_{QS}(t-t_3)} \rho_{QS}^{(n)}(t) d_1^{\dagger} |0\rangle$$
$$+ C_{L02}^{(-)} C_{L13}^{(+)} \langle 0 | e^{-iH_{QS}(t-t_2)} d_1 e^{iH_{QS}(t_1-t_2)} d_1 e^{iH_{QS}(t_3-t_1)} d_1^{\dagger} e^{iH_{QS}(t-t_3)} \rho_{QS}^{(n)}(t) d_1^{\dagger} |0\rangle$$
$$+ C_{L02}^{(-)} C_{R13}^{(+)} \langle 0 | e^{-iH_{QS}(t-t_2)} d_1 e^{iH_{QS}(t_1-t_2)} d_1 e^{iH_{QS}(t_3-t_1)} d_1^{\dagger} e^{iH_{QS}(t-t_3)} \rho_{QS}^{(n)}(t) d_1^{\dagger} |0\rangle$$
$$+ C_{R02}^{(-)} C_{L13}^{(-)} \langle 0 | e^{-iH_{QS}(t-t_2)} d_1 e^{iH_{QS}(t_1-t_2)} d_1^{\dagger} e^{iH_{QS}(t_3-t_1)} d_1 e^{iH_{QS}(t-t_3)} \rho_{QS}^{(n-1)}(t) d_1^{\dagger} |0\rangle$$
$$+ C_{R02}^{(-)} C_{R13}^{(-)} \langle 0 | e^{-iH_{QS}(t-t_2)} d_1 e^{iH_{QS}(t_1-t_2)} d_1^{\dagger} e^{iH_{QS}(t_3-t_1)} d_1 e^{iH_{QS}(t-t_3)} \rho_{QS}^{(n-1)}(t) d_1^{\dagger} |0\rangle$$
$$+ C_{R02}^{(-)} C_{L13}^{(+)} \langle 0 | e^{-iH_{QS}(t-t_2)} d_1 e^{iH_{QS}(t_1-t_2)} d_1 e^{iH_{QS}(t_3-t_1)} d_1^{\dagger} e^{iH_{QS}(t-t_3)} \rho_{QS}^{(n-1)}(t) d_1^{\dagger} |0\rangle$$
$$+ C_{R02}^{(-)} C_{R13}^{(+)} \langle 0 | e^{-iH_{QS}(t-t_2)} d_1 e^{iH_{QS}(t_1-t_2)} d_1 e^{iH_{QS}(t_3-t_1)} d_1^{\dagger} e^{iH_{QS}(t-t_3)} \rho_{QS}^{(n-1)}(t) d_1^{\dagger} |0\rangle \Big]$$
$$+ \text{H.c.}, \tag{I.7}$$

$$\langle 0 | e^{-iH_{QS}t} \rho_{QS,I}(t) \big|_{\text{fourth-order}} e^{iH_{QS}t} \big|_{01,\text{con}} \big|_{04} |0\rangle$$
$$= -\int_{-\infty}^{t} dt_1 \int_{-\infty}^{t_1} dt_2 \int_{-\infty}^{t_2} dt_3$$
$$\times \Big[ C_{L02}^{(-)} C_{L13}^{(+)} \langle 0 | e^{-iH_{QS}(t-t_1)} d_1 e^{iH_{QS}(t_2-t_1)} d_1 e^{iH_{QS}(t_3-t_2)} d_1^{\dagger} e^{iH_{QS}(t-t_3)} \rho_{QS}^{(n)}(t) d_1^{\dagger} |0\rangle$$
$$+ C_{L02}^{(-)} C_{R13}^{(+)} \langle 0 | e^{-iH_{QS}(t-t_1)} d_1 e^{iH_{QS}(t_2-t_1)} d_1 e^{iH_{QS}(t_3-t_2)} d_1^{\dagger} e^{iH_{QS}(t-t_3)} \rho_{QS}^{(n)}(t) d_1^{\dagger} |0\rangle$$
$$+ C_{R02}^{(-)} C_{L13}^{(+)} \langle 0 | e^{-iH_{QS}(t-t_1)} d_1 e^{iH_{QS}(t_2-t_1)} d_1 e^{iH_{QS}(t_3-t_2)} d_1^{\dagger} e^{iH_{QS}(t-t_3)} \rho_{QS}^{(n-1)}(t) d_1^{\dagger} |0\rangle$$
$$+ C_{R02}^{(-)} C_{R13}^{(+)} \langle 0 | e^{-iH_{QS}(t-t_1)} d_1 e^{iH_{QS}(t_2-t_1)} d_1 e^{iH_{QS}(t_3-t_2)} d_1^{\dagger} e^{iH_{QS}(t-t_3)} \rho_{QS}^{(n-1)}(t) d_1^{\dagger} |0\rangle \Big]$$
$$+ \text{H.c.}. \tag{I.8}$$

将 T 型双量子点的电子状态

$$\langle 0 | d_1 = \langle 0, 1 | = a_+ \langle 1 |^{+} + a_- \langle 1 |^{-}, \tag{I.9}$$

代入式 (I.5) 可得

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{01,\mathrm{con}}\Big|_{01}|0\rangle \\
=&\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3 \\
&\times\Big[a_+C_{02}^{(+)}C_{13}^{(-)}\mathrm{e}^{-\mathrm{i}\varepsilon_+(t-t_1)}\langle 1|^+ d_1^\dagger \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t_2-t_1)}d_1^\dagger \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t_3-t_2)}d_1\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_3)}\rho_{\mathrm{QS}}^{(n)}(t)|0\rangle \\
&+a_-C_{02}^{(+)}C_{13}^{(-)}\mathrm{e}^{-\mathrm{i}\varepsilon_-(t-t_1)}\langle 1|^- d_1^\dagger \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t_2-t_1)}d_1^\dagger \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t_3-t_2)}d_1\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_3)}\rho_{\mathrm{QS}}^{(n)}(t)|0\rangle \\
&+a_+C_{02}^{(+)}C_{13}^{(+)}\mathrm{e}^{-\mathrm{i}\varepsilon_+(t-t_1)}\langle 1|^+ d_1 \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t_2-t_1)}d_1^\dagger \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t_3-t_2)}d_1^\dagger\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_3)}\rho_{\mathrm{QS}}^{(n)}(t)|0\rangle \\
&+a_-C_{02}^{(+)}C_{13}^{(+)}\mathrm{e}^{-\mathrm{i}\varepsilon_-(t-t_1)}\langle 1|^- d_1 \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t_2-t_1)}d_1^\dagger \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t_3-t_2)}d_1^\dagger\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_3)}\rho_{\mathrm{QS}}^{(n)}(t)|0\rangle\Big] \\
&+\mathrm{H.c.},
\end{aligned}
\tag{I.10}
$$

然后, 将下面的关系式

$$\langle 1|^+ d_1^\dagger = a_+\langle 0,1|d_1^\dagger + b_+\langle 1,0|d_1^\dagger = a_+\langle 0,0| = a_+\langle 0|, \tag{I.11}$$

$$\langle 1|^- d_1^\dagger = a_-\langle 0,1|d_1^\dagger + b_-\langle 1,0|d_1^\dagger = a_-\langle 0,0| = a_-\langle 0|, \tag{I.12}$$

$$\langle 1|^+ d_1 = a_+\langle 0,1|d_1 + b_+\langle 1,0|d_1 = b_+\langle 1,1|, \tag{I.13}$$

$$\langle 1|^- d_1 = a_-\langle 0,1|d_1 + b_-\langle 1,0|d_1 = b_-\langle 1,1|, \tag{I.14}$$

代入式 (I.10) 可得

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{01,\mathrm{con}}\Big|_{01}|0\rangle \\
=&\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3 \\
&\times\Big[a_+a_+C_{02}^{(+)}C_{13}^{(-)}\mathrm{e}^{-\mathrm{i}\varepsilon_+(t-t_1)}\langle 0|d_1^\dagger \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t_3-t_2)}d_1\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_3)}\rho_{\mathrm{QS}}^{(n)}(t)|0\rangle \\
&+a_-a_-C_{02}^{(+)}C_{13}^{(-)}\mathrm{e}^{-\mathrm{i}\varepsilon_-(t-t_1)}\langle 0|d_1^\dagger \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t_3-t_2)}d_1\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_3)}\rho_{\mathrm{QS}}^{(n)}(t)|0\rangle \\
&+a_+b_+C_{02}^{(+)}C_{13}^{(+)}\mathrm{e}^{-\mathrm{i}\varepsilon_+(t-t_1)}\mathrm{e}^{\mathrm{i}\varepsilon_{1,1}(t_2-t_1)}\langle 1,1|d_1^\dagger \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t_3-t_2)}d_1^\dagger\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_3)}\rho_{\mathrm{QS}}^{(n)}(t)|0\rangle \\
&+a_-b_-C_{02}^{(+)}C_{13}^{(+)}\mathrm{e}^{-\mathrm{i}\varepsilon_-(t-t_1)}\mathrm{e}^{\mathrm{i}\varepsilon_{1,1}(t_2-t_1)}\langle 1,1|d_1^\dagger \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t_3-t_2)}d_1^\dagger\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_3)}\rho_{\mathrm{QS}}^{(n)}(t)|0\rangle\Big] \\
&+\mathrm{H.c.},
\end{aligned}
\tag{I.15}
$$

继续, 将关系式

$$\langle 1,1|d_1^\dagger = \langle 1,0| = b_+\langle 1|^+ + b_-\langle 1|^-, \tag{I.16}$$

代入式 (I.15), 并考虑到 $\langle 0|d_1^\dagger = 0$, 可得

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{01,\mathrm{con}}\Big|_{01}|0\rangle$$

$$
\begin{aligned}
&= \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \\
&\times \Big[ a_+ b_+ b_+ C_{02}^{(+)} C_{13}^{(+)} \mathrm{e}^{-\mathrm{i}\varepsilon_+(t-t_1)} \mathrm{e}^{\mathrm{i}\varepsilon_{1,1}(t_2-t_1)} \mathrm{e}^{\mathrm{i}\varepsilon_+(t_3-t_2)} \langle 1|^+ d_1^\dagger \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_3)} \rho_{\mathrm{QS}}^{(n)}(t) |0\rangle \\
&+ a_+ b_+ b_- C_{02}^{(+)} C_{13}^{(+)} \mathrm{e}^{-\mathrm{i}\varepsilon_+(t-t_1)} \mathrm{e}^{\mathrm{i}\varepsilon_{1,1}(t_2-t_1)} \mathrm{e}^{\mathrm{i}\varepsilon_-(t_3-t_2)} \langle 1|^- d_1^\dagger \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_3)} \rho_{\mathrm{QS}}^{(n)}(t) |0\rangle \\
&+ a_- b_+ b_- C_{02}^{(+)} C_{13}^{(+)} \mathrm{e}^{-\mathrm{i}\varepsilon_-(t-t_1)} \mathrm{e}^{\mathrm{i}\varepsilon_{1,1}(t_2-t_1)} \mathrm{e}^{\mathrm{i}\varepsilon_+(t_3-t_2)} \langle 1|^+ d_1^\dagger \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_3)} \rho_{\mathrm{QS}}^{(n)}(t) |0\rangle \\
&+ a_- b_- b_- C_{02}^{(+)} C_{13}^{(+)} \mathrm{e}^{-\mathrm{i}\varepsilon_-(t-t_1)} \mathrm{e}^{\mathrm{i}\varepsilon_{1,1}(t_2-t_1)} \mathrm{e}^{\mathrm{i}\varepsilon_-(t_3-t_2)} \langle 1|^- d_1^\dagger \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}(t-t_3)} \rho_{\mathrm{QS}}^{(n)}(t) |0\rangle \Big] \\
&+ \mathrm{H.c.}, \qquad \text{(I.17)}
\end{aligned}
$$

最后, 将式 (I.11) 和式 (I.12) 代入式 (I.17) 可得

$$
\begin{aligned}
&\langle 0| \mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t} \rho_{\mathrm{QS,I}}(t) \big|_{\text{fourth-order}} \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t} \big|_{01,\mathrm{con}} \Big|_{01} |0\rangle \\
&= \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \\
&\times \Big[ a_+ a_+ b_+ b_+ C_{02}^{(+)} C_{13}^{(+)} \mathrm{e}^{-\mathrm{i}\varepsilon_+(t-t_1)} \mathrm{e}^{\mathrm{i}\varepsilon_{1,1}(t_2-t_1)} \mathrm{e}^{\mathrm{i}\varepsilon_+(t_3-t_2)} \langle 0| \rho_{\mathrm{QS}}^{(n)}(t) |0\rangle \\
&+ a_+ a_- b_+ b_- C_{02}^{(+)} C_{13}^{(+)} \mathrm{e}^{-\mathrm{i}\varepsilon_+(t-t_1)} \mathrm{e}^{\mathrm{i}\varepsilon_{1,1}(t_2-t_1)} \mathrm{e}^{\mathrm{i}\varepsilon_-(t_3-t_2)} \langle 0| \rho_{\mathrm{QS}}^{(n)}(t) |0\rangle \\
&+ a_+ a_- b_+ b_- C_{02}^{(+)} C_{13}^{(+)} \mathrm{e}^{-\mathrm{i}\varepsilon_-(t-t_1)} \mathrm{e}^{\mathrm{i}\varepsilon_{1,1}(t_2-t_1)} \mathrm{e}^{\mathrm{i}\varepsilon_+(t_3-t_2)} \langle 0| \rho_{\mathrm{QS}}^{(n)}(t) |0\rangle \\
&+ a_- a_- b_- b_- C_{02}^{(+)} C_{13}^{(+)} \mathrm{e}^{-\mathrm{i}\varepsilon_-(t-t_1)} \mathrm{e}^{\mathrm{i}\varepsilon_{1,1}(t_2-t_1)} \mathrm{e}^{\mathrm{i}\varepsilon_-(t_3-t_2)} \langle 0| \rho_{\mathrm{QS}}^{(n)}(t) |0\rangle \Big] \\
&+ \mathrm{H.c.}, \qquad \text{(I.18)}
\end{aligned}
$$

将式 (I.18) 中的指数函数按照时间变量整理可得

$$
\begin{aligned}
&\langle 0| \mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t} \rho_{\mathrm{QS,I}}(t) \big|_{\text{fourth-order}} \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t} \big|_{01,\mathrm{con}} \Big|_{01} |0\rangle \\
&= \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \\
&\times \Big[ a_+ a_+ b_+ b_+ C_{02}^{(+)} C_{13}^{(+)} \mathrm{e}^{-\mathrm{i}\varepsilon_+ t} \mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1} \mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2} \mathrm{e}^{\mathrm{i}\varepsilon_+ t_3} \rho_{\mathrm{QS},00}^{(n)} \\
&+ a_+ a_- b_+ b_- C_{02}^{(+)} C_{13}^{(+)} \mathrm{e}^{-\mathrm{i}\varepsilon_+ t} \mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1} \mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2} \mathrm{e}^{\mathrm{i}\varepsilon_- t_3} \rho_{\mathrm{QS},00}^{(n)} \\
&+ a_+ a_- b_+ b_- C_{02}^{(+)} C_{13}^{(+)} \mathrm{e}^{-\mathrm{i}\varepsilon_- t} \mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1} \mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2} \mathrm{e}^{\mathrm{i}\varepsilon_+ t_3} \rho_{\mathrm{QS},00}^{(n)} \\
&+ a_- a_- b_- b_- C_{02}^{(+)} C_{13}^{(+)} \mathrm{e}^{-\mathrm{i}\varepsilon_- t} \mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1} \mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2} \mathrm{e}^{\mathrm{i}\varepsilon_- t_3} \rho_{\mathrm{QS},00}^{(n)} \Big] + \mathrm{H.c.}, \qquad \text{(I.19)}
\end{aligned}
$$

同理, 式 (I.6)~式 (I.8) 可分别表示为

$$
\begin{aligned}
&\langle 0| \mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t} \rho_{\mathrm{QS,I}}(t) \big|_{\text{fourth-order}} \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t} \big|_{01,\mathrm{con}} \Big|_{02} |0\rangle \\
&= \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3
\end{aligned}
$$

$$\times \Big[ -a_+a_+a_+a_+C_{02}^{(+)}C_{13}^{(+)}\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}\rho_{\mathrm{QS},00}^{(n)}$$
$$- a_+a_+a_-a_-C_{02}^{(+)}C_{13}^{(+)}\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\rho_{\mathrm{QS},00}^{(n)}$$
$$- a_+a_+a_-a_-C_{02}^{(+)}C_{13}^{(+)}\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}\rho_{\mathrm{QS},00}^{(n)}$$
$$-a_-a_-a_-a_-C_{02}^{(+)}C_{13}^{(+)}\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\rho_{\mathrm{QS},00}^{(n)}\Big] + \mathrm{H.c.}, \tag{I.20}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{01,\mathrm{con}}\Big|_{03}|0\rangle\Big|_{01}$$
$$= a_+a_+a_+a_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times\Big[C_{\mathrm{L}02}^{(-)}C_{\mathrm{L}13}^{(-)}\rho_{\mathrm{QS},++}^{(n)} + C_{\mathrm{L}02}^{(-)}C_{\mathrm{R}13}^{(-)}\rho_{\mathrm{QS},++}^{(n)} + C_{\mathrm{R}02}^{(-)}C_{\mathrm{L}13}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)} + C_{\mathrm{R}02}^{(-)}C_{\mathrm{R}13}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}\Big]$$
$$+ a_+a_+a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times\Big[C_{\mathrm{L}02}^{(-)}C_{\mathrm{L}13}^{(-)}\rho_{\mathrm{QS},++}^{(n)} + C_{\mathrm{L}02}^{(-)}C_{\mathrm{R}13}^{(-)}\rho_{\mathrm{QS},++}^{(n)} + C_{\mathrm{R}02}^{(-)}C_{\mathrm{L}13}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)} + C_{\mathrm{R}02}^{(-)}C_{\mathrm{R}13}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}\Big]$$
$$+ a_+a_+b_+b_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}$$
$$\times\Big[C_{\mathrm{L}02}^{(-)}C_{\mathrm{L}13}^{(+)}\rho_{\mathrm{QS},++}^{(n)} + C_{\mathrm{L}02}^{(-)}C_{\mathrm{R}13}^{(+)}\rho_{\mathrm{QS},++}^{(n)} + C_{\mathrm{R}02}^{(-)}C_{\mathrm{L}13}^{(+)}\rho_{\mathrm{QS},++}^{(n-1)} + C_{\mathrm{R}02}^{(-)}C_{\mathrm{R}13}^{(+)}\rho_{\mathrm{QS},++}^{(n-1)}\Big]$$
$$+ a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}$$
$$\times\Big[C_{\mathrm{L}02}^{(-)}C_{\mathrm{L}13}^{(+)}\rho_{\mathrm{QS},++}^{(n)} + C_{\mathrm{L}02}^{(-)}C_{\mathrm{R}13}^{(+)}\rho_{\mathrm{QS},++}^{(n)} + C_{\mathrm{R}02}^{(-)}C_{\mathrm{L}13}^{(+)}\rho_{\mathrm{QS},++}^{(n-1)} + C_{\mathrm{R}02}^{(-)}C_{\mathrm{R}13}^{(+)}\rho_{\mathrm{QS},++}^{(n-1)}\Big]$$
$$+ \mathrm{H.c.}, \tag{I.21-1}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{01,\mathrm{con}}\Big|_{03}|0\rangle\Big|_{02}$$
$$= a_+a_+a_+a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times\Big[C_{\mathrm{L}02}^{(-)}C_{\mathrm{L}13}^{(-)}\rho_{\mathrm{QS},+-}^{(n)} + C_{\mathrm{L}02}^{(-)}C_{\mathrm{R}13}^{(-)}\rho_{\mathrm{QS},+-}^{(n)} + C_{\mathrm{R}02}^{(-)}C_{\mathrm{L}13}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)} + C_{\mathrm{R}02}^{(-)}C_{\mathrm{R}13}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}\Big]$$
$$+ a_+a_-a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times\Big[C_{\mathrm{L}02}^{(-)}C_{\mathrm{L}13}^{(-)}\rho_{\mathrm{QS},+-}^{(n)} + C_{\mathrm{L}02}^{(-)}C_{\mathrm{R}13}^{(-)}\rho_{\mathrm{QS},+-}^{(n)} + C_{\mathrm{R}02}^{(-)}C_{\mathrm{L}13}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)} + C_{\mathrm{R}02}^{(-)}C_{\mathrm{R}13}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}\Big]$$
$$+ a_+a_-b_+b_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}$$
$$\times\Big[C_{\mathrm{L}02}^{(-)}C_{\mathrm{L}13}^{(+)}\rho_{\mathrm{QS},+-}^{(n)} + C_{\mathrm{L}02}^{(-)}C_{\mathrm{R}13}^{(+)}\rho_{\mathrm{QS},+-}^{(n)} + C_{\mathrm{R}02}^{(-)}C_{\mathrm{L}13}^{(+)}\rho_{\mathrm{QS},+-}^{(n-1)} + C_{\mathrm{R}02}^{(-)}C_{\mathrm{R}13}^{(+)}\rho_{\mathrm{QS},+-}^{(n-1)}\Big]$$

$$+ a_- a_- b_+ b_- \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{\mathrm{i}\varepsilon_+ t} \mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1} \mathrm{e}^{-\mathrm{i}\varepsilon_- t_2} \mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}$$
$$\times \left[ C_{\mathrm{L02}}^{(-)} C_{\mathrm{L13}}^{(+)} \rho_{\mathrm{QS},+-}^{(n)} + C_{\mathrm{L02}}^{(-)} C_{\mathrm{R13}}^{(+)} \rho_{\mathrm{QS},+-}^{(n)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{L13}}^{(+)} \rho_{\mathrm{QS},+-}^{(n-1)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{R13}}^{(+)} \rho_{\mathrm{QS},+-}^{(n-1)} \right]$$
$$+ \mathrm{H.c.}, \tag{I.21-2}$$

$$\langle 0| \mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t} \rho_{\mathrm{QS,I}}(t) \Big|_{\text{fourth-order}} \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t} \Big|_{01,\mathrm{con}} \Big|_{03} |0\rangle \Big|_{03}$$
$$= a_+ a_+ a_+ a_- \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{\mathrm{i}\varepsilon_- t} \mathrm{e}^{\mathrm{i}\varepsilon_+ t_1} \mathrm{e}^{-\mathrm{i}\varepsilon_+ t_2} \mathrm{e}^{-\mathrm{i}\varepsilon_- t_3}$$
$$\times \left[ C_{\mathrm{L02}}^{(-)} C_{\mathrm{L13}}^{(-)} \rho_{\mathrm{QS},-+}^{(n)} + C_{\mathrm{L02}}^{(-)} C_{\mathrm{R13}}^{(-)} \rho_{\mathrm{QS},-+}^{(n)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{L13}}^{(-)} \rho_{\mathrm{QS},-+}^{(n-1)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{R13}}^{(-)} \rho_{\mathrm{QS},-+}^{(n-1)} \right]$$
$$+ a_+ a_- a_- a_- \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{\mathrm{i}\varepsilon_- t} \mathrm{e}^{\mathrm{i}\varepsilon_- t_1} \mathrm{e}^{-\mathrm{i}\varepsilon_- t_2} \mathrm{e}^{-\mathrm{i}\varepsilon_- t_3}$$
$$\times \left[ C_{\mathrm{L02}}^{(-)} C_{\mathrm{L13}}^{(-)} \rho_{\mathrm{QS},-+}^{(n)} + C_{\mathrm{L02}}^{(-)} C_{\mathrm{R13}}^{(-)} \rho_{\mathrm{QS},-+}^{(n)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{L13}}^{(-)} \rho_{\mathrm{QS},-+}^{(n-1)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{R13}}^{(-)} \rho_{\mathrm{QS},-+}^{(n-1)} \right]$$
$$+ a_+ a_+ b_+ b_- \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{\mathrm{i}\varepsilon_- t} \mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1} \mathrm{e}^{-\mathrm{i}\varepsilon_+ t_2} \mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}$$
$$\times \left[ C_{\mathrm{L02}}^{(-)} C_{\mathrm{L13}}^{(+)} \rho_{\mathrm{QS},-+}^{(n)} + C_{\mathrm{L02}}^{(-)} C_{\mathrm{R13}}^{(+)} \rho_{\mathrm{QS},-+}^{(n)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{L13}}^{(+)} \rho_{\mathrm{QS},-+}^{(n-1)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{R13}}^{(+)} \rho_{\mathrm{QS},-+}^{(n-1)} \right]$$
$$+ a_+ a_- b_- b_- \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{\mathrm{i}\varepsilon_- t} \mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1} \mathrm{e}^{-\mathrm{i}\varepsilon_- t_2} \mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}$$
$$\times \left[ C_{\mathrm{L02}}^{(-)} C_{\mathrm{L13}}^{(+)} \rho_{\mathrm{QS},-+}^{(n)} + C_{\mathrm{L02}}^{(-)} C_{\mathrm{R13}}^{(+)} \rho_{\mathrm{QS},-+}^{(n)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{L13}}^{(+)} \rho_{\mathrm{QS},-+}^{(n-1)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{R13}}^{(+)} \rho_{\mathrm{QS},-+}^{(n-1)} \right]$$
$$+ \mathrm{H.c.}, \tag{I.21-3}$$

$$\langle 0| \mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t} \rho_{\mathrm{QS,I}}(t) \Big|_{\text{fourth-order}} \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t} \Big|_{01,\mathrm{con}} \Big|_{03} |0\rangle \Big|_{04}$$
$$= a_+ a_+ a_- a_- \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{\mathrm{i}\varepsilon_- t} \mathrm{e}^{\mathrm{i}\varepsilon_+ t_1} \mathrm{e}^{-\mathrm{i}\varepsilon_+ t_2} \mathrm{e}^{-\mathrm{i}\varepsilon_- t_3}$$
$$\times \left[ C_{\mathrm{L02}}^{(-)} C_{\mathrm{L13}}^{(-)} \rho_{\mathrm{QS},--}^{(n)} + C_{\mathrm{L02}}^{(-)} C_{\mathrm{R13}}^{(-)} \rho_{\mathrm{QS},--}^{(n)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{L13}}^{(-)} \rho_{\mathrm{QS},--}^{(n-1)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{R13}}^{(-)} \rho_{\mathrm{QS},--}^{(n-1)} \right]$$
$$+ a_- a_- a_- a_- \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{\mathrm{i}\varepsilon_- t} \mathrm{e}^{\mathrm{i}\varepsilon_- t_1} \mathrm{e}^{-\mathrm{i}\varepsilon_- t_2} \mathrm{e}^{-\mathrm{i}\varepsilon_- t_3}$$
$$\times \left[ C_{\mathrm{L02}}^{(-)} C_{\mathrm{L13}}^{(-)} \rho_{\mathrm{QS},--}^{(n)} + C_{\mathrm{L02}}^{(-)} C_{\mathrm{R13}}^{(-)} \rho_{\mathrm{QS},--}^{(n)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{L13}}^{(-)} \rho_{\mathrm{QS},--}^{(n-1)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{R13}}^{(-)} \rho_{\mathrm{QS},--}^{(n-1)} \right]$$
$$+ a_+ a_- b_+ b_- \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{\mathrm{i}\varepsilon_- t} \mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1} \mathrm{e}^{-\mathrm{i}\varepsilon_+ t_2} \mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}$$
$$\times \left[ C_{\mathrm{L02}}^{(-)} C_{\mathrm{L13}}^{(+)} \rho_{\mathrm{QS},--}^{(n)} + C_{\mathrm{L02}}^{(-)} C_{\mathrm{R13}}^{(+)} \rho_{\mathrm{QS},--}^{(n)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{L13}}^{(+)} \rho_{\mathrm{QS},--}^{(n-1)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{R13}}^{(+)} \rho_{\mathrm{QS},--}^{(n-1)} \right]$$
$$+ a_- a_- b_- b_- \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{\mathrm{i}\varepsilon_- t} \mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1} \mathrm{e}^{-\mathrm{i}\varepsilon_- t_2} \mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}$$

$$\times\left[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L13}}^{(+)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R13}}^{(+)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L13}}^{(+)}\rho_{\mathrm{QS},--}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R13}}^{(+)}\rho_{\mathrm{QS},--}^{(n-1)}\right]$$
$$+\,\mathrm{H.c.}. \tag{I.21-4}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{01,\mathrm{con}}\Big|_{04}|0\rangle\Big|_{01}$$
$$=-a_+a_+b_+b_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}$$
$$\times\left[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L13}}^{(+)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R13}}^{(+)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L13}}^{(+)}\rho_{\mathrm{QS},++}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R13}}^{(+)}\rho_{\mathrm{QS},++}^{(n-1)}\right]$$
$$-a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}$$
$$\times\left[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L13}}^{(+)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R13}}^{(+)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L13}}^{(+)}\rho_{\mathrm{QS},++}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R13}}^{(+)}\rho_{\mathrm{QS},++}^{(n-1)}\right]$$
$$+\,\mathrm{H.c.}, \tag{I.22-1}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{01,\mathrm{con}}\Big|_{04}|0\rangle\Big|_{02}$$
$$=-a_+a_-b_+b_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}$$
$$\times\left[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L13}}^{(+)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R13}}^{(+)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L13}}^{(+)}\rho_{\mathrm{QS},+-}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R13}}^{(+)}\rho_{\mathrm{QS},+-}^{(n-1)}\right]$$
$$-a_-a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}$$
$$\times\left[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L13}}^{(+)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R13}}^{(+)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L13}}^{(+)}\rho_{\mathrm{QS},+-}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R13}}^{(+)}\rho_{\mathrm{QS},+-}^{(n-1)}\right]$$
$$+\,\mathrm{H.c.}, \tag{I.22-2}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{01,\mathrm{con}}\Big|_{04}|0\rangle\Big|_{03}$$
$$=-a_+a_+b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}$$
$$\times\left[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L13}}^{(+)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R13}}^{(+)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L13}}^{(+)}\rho_{\mathrm{QS},-+}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R13}}^{(+)}\rho_{\mathrm{QS},-+}^{(n-1)}\right]$$
$$-a_+a_-b_-b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}$$
$$\times\left[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L13}}^{(+)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R13}}^{(+)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L13}}^{(+)}\rho_{\mathrm{QS},-+}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R13}}^{(+)}\rho_{\mathrm{QS},-+}^{(n-1)}\right]$$
$$+\,\mathrm{H.c.}, \tag{I.22-3}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{01,\mathrm{con}}\Big|_{04}|0\rangle\Big|_{04}$$

$$
\begin{aligned}
&= -a_+a_-b_+b_- \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{\mathrm{i}\varepsilon_- t} \mathrm{e}^{-\mathrm{i}\varepsilon_+ t_1} \mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2} \mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3} \\
&\quad \times \left[ C_{\mathrm{L02}}^{(-)} C_{\mathrm{L13}}^{(+)} \rho_{\mathrm{QS},--}^{(n)} + C_{\mathrm{L02}}^{(-)} C_{\mathrm{R13}}^{(+)} \rho_{\mathrm{QS},--}^{(n)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{L13}}^{(+)} \rho_{\mathrm{QS},--}^{(n-1)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{R13}}^{(+)} \rho_{\mathrm{QS},--}^{(n-1)} \right] \\
&\quad - a_-a_-b_-b_- \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{\mathrm{i}\varepsilon_- t} \mathrm{e}^{-\mathrm{i}\varepsilon_- t_1} \mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2} \mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3} \\
&\quad \times \left[ C_{\mathrm{L02}}^{(-)} C_{\mathrm{L13}}^{(+)} \rho_{\mathrm{QS},--}^{(n)} + C_{\mathrm{L02}}^{(-)} C_{\mathrm{R13}}^{(+)} \rho_{\mathrm{QS},--}^{(n)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{L13}}^{(+)} \rho_{\mathrm{QS},--}^{(n-1)} + C_{\mathrm{R02}}^{(-)} C_{\mathrm{R13}}^{(+)} \rho_{\mathrm{QS},--}^{(n-1)} \right] \\
&\quad + \mathrm{H.c.}. \qquad \text{(I.22-4)}
\end{aligned}
$$

对于 $\dot{\rho}_{\mathrm{S,co},00}^{(n)}(t)$ 的第二部分，由式 (G.1)~式 (G.4) 可得

$$
\begin{aligned}
&\langle 0| \mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t} \rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}} \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{02,\mathrm{con}}\Big|_{01} |0\rangle\Big|_{01} \\
&= a_+a_+a_+a_+ \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{-\mathrm{i}\varepsilon_+ t} \mathrm{e}^{-\mathrm{i}\varepsilon_+ t_1} \mathrm{e}^{\mathrm{i}\varepsilon_+ t_2} \mathrm{e}^{\mathrm{i}\varepsilon_+ t_3} \\
&\quad \times \left[ C_{\mathrm{L02}}^{(+)} C_{\mathrm{L31}}^{(-)} \rho_{\mathrm{QS},++}^{(n)} + C_{\mathrm{R02}}^{(+)} C_{\mathrm{L31}}^{(-)} \rho_{\mathrm{QS},++}^{(n)} + C_{\mathrm{L02}}^{(+)} C_{\mathrm{R31}}^{(-)} \rho_{\mathrm{QS},++}^{(n-1)} + C_{\mathrm{R02}}^{(+)} C_{\mathrm{R31}}^{(-)} \rho_{\mathrm{QS},++}^{(n-1)} \right] \\
&\quad + a_+a_+a_-a_- \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{-\mathrm{i}\varepsilon_- t} \mathrm{e}^{-\mathrm{i}\varepsilon_+ t_1} \mathrm{e}^{\mathrm{i}\varepsilon_- t_2} \mathrm{e}^{\mathrm{i}\varepsilon_+ t_3} \\
&\quad \times \left[ C_{\mathrm{L02}}^{(+)} C_{\mathrm{L31}}^{(-)} \rho_{\mathrm{QS},++}^{(n)} + C_{\mathrm{R02}}^{(+)} C_{\mathrm{L31}}^{(-)} \rho_{\mathrm{QS},++}^{(n)} + C_{\mathrm{L02}}^{(+)} C_{\mathrm{R31}}^{(-)} \rho_{\mathrm{QS},++}^{(n-1)} + C_{\mathrm{R02}}^{(+)} C_{\mathrm{R31}}^{(-)} \rho_{\mathrm{QS},++}^{(n-1)} \right] \\
&\quad + \mathrm{H.c.}, \qquad \text{(I.23-1)}
\end{aligned}
$$

$$
\begin{aligned}
&\langle 0| \mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t} \rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}} \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{02,\mathrm{con}}\Big|_{01} |0\rangle\Big|_{02} \\
&= a_+a_+a_+a_- \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{-\mathrm{i}\varepsilon_- t} \mathrm{e}^{-\mathrm{i}\varepsilon_+ t_1} \mathrm{e}^{\mathrm{i}\varepsilon_+ t_2} \mathrm{e}^{\mathrm{i}\varepsilon_- t_3} \\
&\quad \times \left[ C_{\mathrm{L02}}^{(+)} C_{\mathrm{L31}}^{(-)} \rho_{\mathrm{QS},+-}^{(n)} + C_{\mathrm{R02}}^{(+)} C_{\mathrm{L31}}^{(-)} \rho_{\mathrm{QS},+-}^{(n)} + C_{\mathrm{L02}}^{(+)} C_{\mathrm{R31}}^{(-)} \rho_{\mathrm{QS},+-}^{(n-1)} + C_{\mathrm{R02}}^{(+)} C_{\mathrm{R31}}^{(-)} \rho_{\mathrm{QS},+-}^{(n-1)} \right] \\
&\quad + a_+a_-a_-a_- \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{\mathrm{i}(\varepsilon_+-2\varepsilon_-)t} \mathrm{e}^{-\mathrm{i}\varepsilon_+ t_1} \mathrm{e}^{\mathrm{i}\varepsilon_- t_2} \mathrm{e}^{\mathrm{i}\varepsilon_- t_3} \\
&\quad \times \left[ C_{\mathrm{L02}}^{(+)} C_{\mathrm{L31}}^{(-)} \rho_{\mathrm{QS},+-}^{(n)} + C_{\mathrm{R02}}^{(+)} C_{\mathrm{L31}}^{(-)} \rho_{\mathrm{QS},+-}^{(n)} + C_{\mathrm{L02}}^{(+)} C_{\mathrm{R31}}^{(-)} \rho_{\mathrm{QS},+-}^{(n-1)} + C_{\mathrm{R02}}^{(+)} C_{\mathrm{R31}}^{(-)} \rho_{\mathrm{QS},+-}^{(n-1)} \right] \\
&\quad + \mathrm{H.c.}, \qquad \text{(I.23-2)}
\end{aligned}
$$

$$
\begin{aligned}
&\langle 0| \mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t} \rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}} \mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{02,\mathrm{con}}\Big|_{01} |0\rangle\Big|_{03} \\
&= a_+a_+a_+a_- \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{\mathrm{i}(\varepsilon_--2\varepsilon_+)t} \mathrm{e}^{-\mathrm{i}\varepsilon_- t_1} \mathrm{e}^{\mathrm{i}\varepsilon_+ t_2} \mathrm{e}^{\mathrm{i}\varepsilon_+ t_3} \\
&\quad \times \left[ C_{\mathrm{L02}}^{(+)} C_{\mathrm{L31}}^{(-)} \rho_{\mathrm{QS},-+}^{(n)} + C_{\mathrm{R02}}^{(+)} C_{\mathrm{L31}}^{(-)} \rho_{\mathrm{QS},-+}^{(n)} + C_{\mathrm{L02}}^{(+)} C_{\mathrm{R31}}^{(-)} \rho_{\mathrm{QS},-+}^{(n-1)} + C_{\mathrm{R02}}^{(+)} C_{\mathrm{R31}}^{(-)} \rho_{\mathrm{QS},-+}^{(n-1)} \right]
\end{aligned}
$$

$$
\begin{aligned}
&+a_+a_-a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}\\
&\times\left[C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}\right]\\
&+\mathrm{H.c.},
\end{aligned}\tag{I.23-3}
$$

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{02,\mathrm{con}}\Big|_{01}|0\rangle\Big|_{04}\\
=&\,a_+a_+a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\\
&\times\left[C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}\right]\\
&+a_-a_-a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\\
&\times\left[C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}\right]\\
&+\mathrm{H.c.}.
\end{aligned}\tag{I.23-4}
$$

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{02,\mathrm{con}}\Big|_{02}|0\rangle\Big|_{01}\\
=&-a_+a_+b_+b_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}\\
&\times\left[C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}\right]\\
&-a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}\\
&\times\left[C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}\right]\\
&+\mathrm{H.c.},
\end{aligned}\tag{I.24-1}
$$

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{02,\mathrm{con}}\Big|_{02}|0\rangle\Big|_{02}\\
=&-a_+a_-b_+b_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\\
&\times\left[C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}\right]\\
&-a_-a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}(\varepsilon_+-2\varepsilon_-)t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\\
&\times\left[C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}\right]\\
&+\mathrm{H.c.},
\end{aligned}\tag{I.24-2}
$$

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\Big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{02,\mathrm{con}}\Big|_{02}|0\rangle\Big|_{03}\\
=&-a_+a_+b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}(\varepsilon_--2\varepsilon_+)t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}\\
&\times\left[C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}\right]\\
&-a_+a_-b_-b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}\\
&\times\left[C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}\right]\\
&+\mathrm{H.c.},
\end{aligned}\tag{I.24-3}
$$

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\Big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{02,\mathrm{con}}\Big|_{02}|0\rangle\Big|_{04}\\
=&-a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\\
&\times\left[C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}\right]\\
&-a_-a_-b_-b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\\
&\times\left[C_{\mathrm{L02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{L02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}+C_{\mathrm{R02}}^{(+)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}\right]\\
&+\mathrm{H.c.}.
\end{aligned}\tag{I.24-4}
$$

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\Big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{02,\mathrm{con}}\Big|_{03}|0\rangle\Big|_{01}\\
=&\,a_+a_+b_+b_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}\\
&\times\left[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\right]\\
&+a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}\\
&\times\left[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\right]\\
&+\mathrm{H.c.},
\end{aligned}\tag{I.25-1}
$$

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\Big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{02,\mathrm{con}}\Big|_{03}|0\rangle\Big|_{02}\\
=&\,a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}\\
&\times\left[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\right]
\end{aligned}
$$

$$+\,a_-a_-b_-b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}$$
$$\times\Big[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\Big]$$
$$+\,\mathrm{H.c.}. \tag{I.25-2}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{02,\mathrm{con}}\Big|_{04}|0\rangle\Big|_{01}$$
$$=-a_+a_+a_+a_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times\left[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(+)}\rho_{\mathrm{QS},00}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(+)}\rho_{\mathrm{QS},00}^{(n+1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(+)}\rho_{\mathrm{QS},00}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(+)}\rho_{\mathrm{QS},00}^{(n)}\right]$$
$$-\,a_+a_+a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}$$
$$\times\left[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(+)}\rho_{\mathrm{QS},00}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(+)}\rho_{\mathrm{QS},00}^{(n+1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(+)}\rho_{\mathrm{QS},00}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(+)}\rho_{\mathrm{QS},00}^{(n)}\right]$$
$$+\,\mathrm{H.c.}, \tag{I.26-1}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{02,\mathrm{con}}\Big|_{04}|0\rangle\Big|_{02}$$
$$=-a_+a_+a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times\left[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(+)}\rho_{\mathrm{QS},00}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(+)}\rho_{\mathrm{QS},00}^{(n+1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(+)}\rho_{\mathrm{QS},00}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(+)}\rho_{\mathrm{QS},00}^{(n)}\right]$$
$$-\,a_-a_-a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}$$
$$\times\left[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(+)}\rho_{\mathrm{QS},00}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(+)}\rho_{\mathrm{QS},00}^{(n+1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(+)}\rho_{\mathrm{QS},00}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(+)}\rho_{\mathrm{QS},00}^{(n)}\right]$$
$$+\,\mathrm{H.c.}, \tag{I.26-2}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{02,\mathrm{con}}\Big|_{04}|0\rangle\Big|_{03}$$
$$=-a_+a_+b_+b_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}$$
$$\times\Big[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\Big]$$
$$-\,a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}$$
$$\times\Big[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\Big]$$
$$+\,\mathrm{H.c.}, \tag{I.26-3}$$

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{02,\mathrm{con}}\Big|_{04}|0\rangle\Big|_{04}\\
=&-a_+a_-b_+b_-\sum_{ijkl}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}\\
&\times\Big[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\Big]\\
&-a_-a_-b_-b_-\sum_{ijkl}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}\\
&\times\Big[C_{\mathrm{L02}}^{(-)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L02}}^{(-)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{L31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R02}}^{(-)}C_{\mathrm{R31}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\Big]\\
&+\mathrm{H.c.}. \qquad\qquad (\mathrm{I.26\text{-}4})
\end{aligned}
$$

对于 $\dot{\rho}_{\mathrm{S,co},00}^{(n)}(t)$ 的第三部分，由式 (G.5)~式 (G.8) 可得

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{03,\mathrm{con}}\Big|_{01}|0\rangle\\
=&\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\\
&\times\Big[a_+a_+a_+a_+C_{03}^{(+)}C_{12}^{(-)}\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}\rho_{\mathrm{QS},00}^{(n)}\\
&+a_+a_+a_-a_-C_{03}^{(+)}C_{12}^{(-)}\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}\rho_{\mathrm{QS},00}^{(n)}\\
&+a_+a_+a_-a_-C_{03}^{(+)}C_{12}^{(-)}\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\rho_{\mathrm{QS},00}^{(n)}\\
&+a_-a_-a_-a_-C_{03}^{(+)}C_{12}^{(-)}\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\rho_{\mathrm{QS},00}^{(n)}\\
&+a_+a_+b_+b_+C_{03}^{(+)}C_{12}^{(+)}\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}\rho_{\mathrm{QS},00}^{(n)}\\
&+a_+a_-b_+b_-C_{03}^{(+)}C_{12}^{(+)}\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}\rho_{\mathrm{QS},00}^{(n)}\\
&+a_+a_-b_+b_-C_{03}^{(+)}C_{12}^{(+)}\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\rho_{\mathrm{QS},00}^{(n)}\\
&+a_-a_-b_-b_-C_{03}^{(+)}C_{12}^{(+)}\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\rho_{\mathrm{QS},00}^{(n)}\Big]\\
&+\mathrm{H.c.}. \qquad\qquad (\mathrm{I.27})
\end{aligned}
$$

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{03,\mathrm{con}}\Big|_{02}|0\rangle\\
=&-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\\
&\times\Big[C_{03}^{(+)}C_{12}^{(+)}a_+a_+a_+a_+\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}\rho_{\mathrm{QS},00}^{(n)}\\
&+C_{03}^{(+)}C_{12}^{(+)}a_+a_+a_-a_-\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\rho_{\mathrm{QS},00}^{(n)}
\end{aligned}
$$

$$+C_{03}^{(+)}C_{12}^{(+)}a_+a_+a_-a_-\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}\rho_{\mathrm{QS},00}^{(n)}$$
$$+C_{03}^{(+)}C_{12}^{(+)}a_-a_-a_-a_-\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\rho_{\mathrm{QS},00}^{(n)}\Big]+\mathrm{H.c.}. \tag{I.28}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{03,\mathrm{con}}\Big|_{03}|0\rangle\Big|_{01}$$
$$=a_+a_+a_+a_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times\Big[C_{\mathrm{L}03}^{(-)}C_{\mathrm{L}12}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{L}03}^{(-)}C_{\mathrm{R}12}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{L}12}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{R}12}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}\Big]$$
$$+a_+a_+a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}$$
$$\times\Big[C_{\mathrm{L}03}^{(-)}C_{\mathrm{L}12}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{L}03}^{(-)}C_{\mathrm{R}12}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{L}12}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{R}12}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}\Big]$$
$$+a_+a_+b_+b_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times\Big[C_{\mathrm{L}03}^{(-)}C_{\mathrm{L}12}^{(+)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{L}03}^{(-)}C_{\mathrm{R}12}^{(+)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{L}12}^{(+)}\rho_{\mathrm{QS},++}^{(n-1)}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{R}12}^{(+)}\rho_{\mathrm{QS},++}^{(n-1)}\Big]$$
$$+a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}$$
$$\times\Big[C_{\mathrm{L}03}^{(-)}C_{\mathrm{L}12}^{(+)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{L}03}^{(-)}C_{\mathrm{R}12}^{(+)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{L}12}^{(+)}\rho_{\mathrm{QS},++}^{(n-1)}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{R}12}^{(+)}\rho_{\mathrm{QS},++}^{(n-1)}\Big]$$
$$+\mathrm{H.c.}, \tag{I.29-1}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{03,\mathrm{con}}\Big|_{03}|0\rangle\Big|_{02}$$
$$=a_+a_+a_+a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times\Big[C_{\mathrm{L}03}^{(-)}C_{\mathrm{L}12}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{L}03}^{(-)}C_{\mathrm{R}12}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{L}12}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{R}12}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}\Big]$$
$$+a_+a_-a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}$$
$$\times\Big[C_{\mathrm{L}03}^{(-)}C_{\mathrm{L}12}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{L}03}^{(-)}C_{\mathrm{R}12}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{L}12}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{R}12}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}\Big]$$
$$+a_+a_-b_+b_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times\Big[C_{\mathrm{L}03}^{(-)}C_{\mathrm{L}12}^{(+)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{L}03}^{(-)}C_{\mathrm{R}12}^{(+)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{L}12}^{(+)}\rho_{\mathrm{QS},+-}^{(n-1)}+C_{\mathrm{R}03}^{(-)}C_{\mathrm{R}12}^{(+)}\rho_{\mathrm{QS},+-}^{(n-1)}\Big]$$
$$+a_-a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}$$

$$\times \left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},+-}^{(n)} + C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},+-}^{(n)} + C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},+-}^{(n-1)} + C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},+-}^{(n-1)}\right]$$
$$+ \mathrm{H.c.}, \tag{I.29-2}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{03,\mathrm{con}}\Big|_{03}|0\rangle\Big|_{03}$$
$$= a_+a_+a_+a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times \left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)} + C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)} + C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)} + C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}\right]$$
$$+ a_+a_-a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}$$
$$\times \left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)} + C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)} + C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)} + C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}\right]$$
$$+ a_+a_+b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times \left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},-+}^{(n)} + C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},-+}^{(n)} + C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},-+}^{(n-1)} + C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},-+}^{(n-1)}\right]$$
$$+ a_+a_-b_-b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}$$
$$\times \left\{C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},-+}^{(n)} + C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},-+}^{(n)} + C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},-+}^{(n-1)} + C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},-+}^{(n-1)}\right\}$$
$$+ \mathrm{H.c.}, \tag{I.29-3}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{03,\mathrm{con}}\Big|_{03}|0\rangle\Big|_{04}$$
$$= a_+a_+a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times \left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},--}^{(n)} + C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},--}^{(n)} + C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)} + C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}\right]$$
$$+ a_-a_-a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}$$
$$\times \left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},--}^{(n)} + C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},--}^{(n)} + C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)} + C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}\right]$$
$$+ a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times \left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},--}^{(n)} + C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},--}^{(n)} + C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},--}^{(n-1)} + C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},--}^{(n-1)}\right]$$
$$+ a_-a_-b_-b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}$$

$$\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},--}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},--}^{(n-1)}\right]$$
$$+\,\mathrm{H.c.}. \tag{I.29-4}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{03,\mathrm{con}}\Big|_{04}|0\rangle\Big|_{01}$$
$$=-a_+a_+a_+a_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},++}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},++}^{(n-1)}\right]$$
$$-\,a_+a_+a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},++}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},++}^{(n-1)}\right]$$
$$+\,\mathrm{H.c.}, \tag{I.30-1}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{03,\mathrm{con}}\Big|_{04}|0\rangle\Big|_{02}$$
$$=-a_+a_+a_+a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},+-}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},+-}^{(n-1)}\right]$$
$$-\,a_+a_-a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},+-}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},+-}^{(n-1)}\right]$$
$$+\,\mathrm{H.c.}, \tag{I.30-2}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{03,\mathrm{con}}\Big|_{04}|0\rangle\Big|_{03}$$
$$=-a_+a_+a_+a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},-+}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},-+}^{(n-1)}\right]$$
$$-\,a_+a_-a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},-+}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},-+}^{(n-1)}\right]$$
$$+\,\mathrm{H.c.}, \tag{I.30-3}$$

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\Big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{03,\mathrm{con}}\Big|_{04}|0\rangle\Big|_{04}\\
=&-a_+a_+a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}\\
&\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},--}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},--}^{(n-1)}\right]\\
&-a_-a_-a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}\\
&\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},--}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},--}^{(n-1)}\right]\\
&+\mathrm{H.c.}. \qquad\qquad \text{(I.30-4)}
\end{aligned}
$$

对于 $\dot{\rho}_{\mathrm{S,co,00}}^{(n)}(t)$ 的第四部分，由式 (G.9)~式 (G.12) 可得

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\Big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{04,\mathrm{con}}\Big|_{01}|0\rangle\Big|_{01}\\
=&a_+a_+a_+a_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}\\
&\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}\right]\\
&+a_+a_+a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\\
&\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}\right]\\
&+\mathrm{H.c.}, \qquad\qquad \text{(I.31-1)}
\end{aligned}
$$

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\Big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{04,\mathrm{con}}\Big|_{01}|0\rangle\Big|_{02}\\
=&a_+a_+a_+a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}\\
&\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}\right]\\
&+a_+a_-a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}(\varepsilon_+-2\varepsilon_-)t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\\
&\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}\right]\\
&+\mathrm{H.c.}, \qquad\qquad \text{(I.31-2)}
\end{aligned}
$$

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\Big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{04,\mathrm{con}}\Big|_{01}|0\rangle\Big|_{03}\\
=&a_+a_+a_+a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}(\varepsilon_--2\varepsilon_+)t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}
\end{aligned}
$$

$$\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}\right]$$
$$+a_+a_-a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}\right]$$
$$+\mathrm{H.c.},\tag{I.31-3}$$

$$\begin{aligned}&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{04,\mathrm{con}}\Big|_{01}|0\rangle\Big|_{04}\\
=&\,a_+a_+a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}\\
&\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}\right]\\
&+a_-a_-a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\\
&\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}\right]\\
&+\mathrm{H.c.}.\end{aligned}\tag{I.31-4}$$

$$\begin{aligned}&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{04,\mathrm{con}}\Big|_{02}|0\rangle\Big|_{01}\\
=&-a_+a_+b_+b_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}\\
&\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}\right]\\
&-a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}\\
&\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}\right]\\
&+\mathrm{H.c.},\end{aligned}\tag{I.32-1}$$

$$\begin{aligned}&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{04,\mathrm{con}}\Big|_{02}|0\rangle\Big|_{02}\\
=&-a_+a_-b_+b_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}\\
&\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}\right]\\
&-a_-a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}(\varepsilon_+-2\varepsilon_-)t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}\\
&\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}\right]\end{aligned}$$

$$+\,\mathrm{H.c.},\tag{I.32-2}$$

$$\begin{aligned}
&\left.\left.\left\langle 0\right|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\right|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{04,\mathrm{con}}\Big|_{02}\left|0\right\rangle\right|_{03}\\
=&-a_+a_+b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}(\varepsilon_--2\varepsilon_+)t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}\\
&\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}\right]\\
&-a_+a_-b_-b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}\\
&\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}\right]\\
&+\mathrm{H.c.},
\end{aligned}\tag{I.32-3}$$

$$\begin{aligned}
&\left.\left.\left\langle 0\right|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\right|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{04,\mathrm{con}}\Big|_{02}\left|0\right\rangle\right|_{04}\\
=&-a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}\\
&\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}\right]\\
&-a_-a_-b_-b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}\\
&\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}\right]\\
&+\mathrm{H.c.}.
\end{aligned}\tag{I.32-4}$$

$$\begin{aligned}
&\left.\left\langle 0\right|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\right|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{04,\mathrm{con}}\Big|_{03}\left|0\right\rangle\\
=&\,a_+a_+b_+b_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}\\
&\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\right]\\
&+a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}\\
&\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\right]\\
&+a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}\\
&\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\right]\\
&+a_-a_-b_-b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}
\end{aligned}$$

$$\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\right]$$
$$+\,\mathrm{H.c.}, \tag{I.33}$$

$$\left.\left.\left.\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\right|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\right|_{04,\mathrm{con}}\right|_{04}|0\rangle\Big|_{01}$$
$$=-a_+a_+a_+a_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},00}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},00}^{(n+1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},00}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},00}^{(n)}\right]$$
$$-a_+a_+a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},00}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},00}^{(n+1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},00}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},00}^{(n)}\right]$$
$$+\,\mathrm{H.c.}, \tag{I.34-1}$$

$$\left.\left.\left.\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\right|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\right|_{04,\mathrm{con}}\right|_{04}|0\rangle\Big|_{02}$$
$$=-a_+a_+a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},00}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},00}^{(n+1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},00}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},00}^{(n)}\right]$$
$$-a_-a_-a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},00}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},00}^{(n+1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(+)}\rho_{\mathrm{QS},00}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(+)}\rho_{\mathrm{QS},00}^{(n)}\right]$$
$$+\,\mathrm{H.c.}, \tag{I.34-2}$$

$$\left.\left.\left.\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\right|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\right|_{04,\mathrm{con}}\right|_{04}|0\rangle\Big|_{03}$$
$$=-a_+a_+b_+b_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\right]$$
$$-a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\right]$$
$$+\,\mathrm{H.c.}, \tag{I.34-3}$$

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{04,\mathrm{con}}\Big|_{04}|0\rangle\Big|_{04}\\
=&-a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}\\
&\times\Big[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\Big]\\
&-a_-a_-b_-b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}\\
&\times\Big[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R12}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\Big]\\
&+\mathrm{H.c.}.
\end{aligned}\tag{I.34-4}
$$

对于 $\dot{\rho}_{\mathrm{S,co},00}^{(n)}(t)$ 的第五部分，由式 (G.13)~式 (G.16) 可得

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{05,\mathrm{con}}\Big|_{01}|0\rangle\Big|_{01}\\
=&\,a_+a_+a_+a_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}\\
&\times\Big[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}\Big]\\
&+a_+a_+a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\\
&\times\Big[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}\Big]\\
&+\mathrm{H.c.},
\end{aligned}\tag{I.35-1}
$$

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{05,\mathrm{con}}\Big|_{01}|0\rangle\Big|_{02}\\
=&\,a_+a_+a_+a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}\\
&\times\Big[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}\Big]\\
&+a_+a_-a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}(\varepsilon_+-2\varepsilon_-)t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}\\
&\times\Big[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}\Big]\\
&+\mathrm{H.c.},
\end{aligned}\tag{I.35-2}
$$

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{05,\mathrm{con}}\Big|_{01}|0\rangle\Big|_{03}\\
=&\,a_+a_+a_+a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}(\varepsilon_--2\varepsilon_+)t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}
\end{aligned}
$$

$$\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}\right]$$
$$+a_+a_-a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}\right]$$
$$+\mathrm{H.c.},\tag{I.35-3}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{05,\mathrm{con}}\Big|_{01}|0\rangle\Big|_{04}$$
$$=a_+a_+a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}\varepsilon_+t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}\right]$$
$$+a_-a_-a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}\varepsilon_-t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}\right]$$
$$+\mathrm{H.c.}.\tag{I.35-4}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{05,\mathrm{con}}\Big|_{02}|0\rangle\Big|_{01}$$
$$=-a_+a_+b_+b_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}\right]$$
$$-a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},++}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},++}^{(n-1)}\right]$$
$$+\mathrm{H.c.},\tag{I.36-1}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{05,\mathrm{con}}\Big|_{02}|0\rangle\Big|_{02}$$
$$=-a_+a_-b_+b_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}\right]$$
$$-a_-a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}(\varepsilon_+-2\varepsilon_-)t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}$$
$$\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},+-}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},+-}^{(n-1)}\right]$$

$$+\text{H.c.},\tag{I.36-2}$$

$$\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{05,\mathrm{con}}\Big|_{02}|0\rangle\Big|_{03}\\
=&-a_+a_+b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}(\varepsilon_- -2\varepsilon_+)t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}\\
&\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}\right]\\
&-a_+a_-b_-b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}\\
&\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},-+}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},-+}^{(n-1)}\right]\\
&+\text{H.c.},
\end{aligned}\tag{I.36-3}$$

$$\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{05,\mathrm{con}}\Big|_{02}|0\rangle\Big|_{04}\\
=&-a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}\\
&\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}\right]\\
&-a_-a_-b_-b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}\\
&\times\left[C_{\mathrm{L03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{L03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},--}^{(n)}+C_{\mathrm{R03}}^{(+)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},--}^{(n-1)}\right]\\
&+\text{H.c.}.
\end{aligned}\tag{I.36-4}$$

$$\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{05,\mathrm{con}}\Big|_{03}|0\rangle\Big|_{01}\\
=&\,a_+a_+b_+b_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}\\
&\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\right]\\
&+a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}\\
&\times\left[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\right]\\
&+\text{H.c.},
\end{aligned}\tag{I.37-1}$$

$$\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\,\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{05,\mathrm{con}}\Big|_{03}|0\rangle\Big|_{02}\\
=&\,a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_3}
\end{aligned}$$

$$\times\Big[C^{(-)}_{\mathrm{L03}}C^{(-)}_{\mathrm{L21}}\rho^{(n)}_{\mathrm{QS},11,11}+C^{(-)}_{\mathrm{L03}}C^{(-)}_{\mathrm{R21}}\rho^{(n-1)}_{\mathrm{QS},11,11}+C^{(-)}_{\mathrm{R03}}C^{(-)}_{\mathrm{L21}}\rho^{(n-1)}_{\mathrm{QS},11,11}+C^{(-)}_{\mathrm{R03}}C^{(-)}_{\mathrm{R21}}\rho^{(n-2)}_{\mathrm{QS},11,11}\Big]$$

$$+a_-a_-b_-b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_3}$$

$$\times\Big[C^{(-)}_{\mathrm{L03}}C^{(-)}_{\mathrm{L21}}\rho^{(n)}_{\mathrm{QS},11,11}+C^{(-)}_{\mathrm{L03}}C^{(-)}_{\mathrm{R21}}\rho^{(n-1)}_{\mathrm{QS},11,11}+C^{(-)}_{\mathrm{R03}}C^{(-)}_{\mathrm{L21}}\rho^{(n-1)}_{\mathrm{QS},11,11}+C^{(-)}_{\mathrm{R03}}C^{(-)}_{\mathrm{R21}}\rho^{(n-2)}_{\mathrm{QS},11,11}\Big]$$

$$+\,\mathrm{H.c.},\tag{I.37-2}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{05,\mathrm{con}}\Big|_{04}|0\rangle\Big|_{01}$$

$$=-a_+a_+a_+a_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$

$$\times\left[C^{(-)}_{\mathrm{L03}}C^{(+)}_{\mathrm{L21}}\rho^{(n)}_{\mathrm{QS},00}+C^{(-)}_{\mathrm{L03}}C^{(+)}_{\mathrm{R21}}\rho^{(n+1)}_{\mathrm{QS},00}+C^{(-)}_{\mathrm{R03}}C^{(+)}_{\mathrm{L21}}\rho^{(n-1)}_{\mathrm{QS},00}+C^{(-)}_{\mathrm{R03}}C^{(+)}_{\mathrm{R21}}\rho^{(n)}_{\mathrm{QS},00}\right]$$

$$-a_+a_+a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}$$

$$\times\left[C^{(-)}_{\mathrm{L03}}C^{(+)}_{\mathrm{L21}}\rho^{(n)}_{\mathrm{QS},00}+C^{(-)}_{\mathrm{L03}}C^{(+)}_{\mathrm{R21}}\rho^{(n+1)}_{\mathrm{QS},00}+C^{(-)}_{\mathrm{R03}}C^{(+)}_{\mathrm{L21}}\rho^{(n-1)}_{\mathrm{QS},00}+C^{(-)}_{\mathrm{R03}}C^{(+)}_{\mathrm{R21}}\rho^{(n)}_{\mathrm{QS},00}\right]$$

$$+\,\mathrm{H.c.},\tag{I.38-1}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{05,\mathrm{con}}\Big|_{04}|0\rangle\Big|_{02}$$

$$=-a_+a_+a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}\varepsilon_+t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$

$$\times\left[C^{(-)}_{\mathrm{L03}}C^{(+)}_{\mathrm{L21}}\rho^{(n)}_{\mathrm{QS},00}+C^{(-)}_{\mathrm{L03}}C^{(+)}_{\mathrm{R21}}\rho^{(n+1)}_{\mathrm{QS},00}+C^{(-)}_{\mathrm{R03}}C^{(+)}_{\mathrm{L21}}\rho^{(n-1)}_{\mathrm{QS},00}+C^{(-)}_{\mathrm{R03}}C^{(+)}_{\mathrm{R21}}\rho^{(n)}_{\mathrm{QS},00}\right]$$

$$-a_-a_-a_-a_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{\mathrm{i}\varepsilon_-t_1}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}$$

$$\times\left[C^{(-)}_{\mathrm{L03}}C^{(+)}_{\mathrm{L21}}\rho^{(n)}_{\mathrm{QS},00}+C^{(-)}_{\mathrm{L03}}C^{(+)}_{\mathrm{R21}}\rho^{(n+1)}_{\mathrm{QS},00}+C^{(-)}_{\mathrm{R03}}C^{(+)}_{\mathrm{L21}}\rho^{(n-1)}_{\mathrm{QS},00}+C^{(-)}_{\mathrm{R03}}C^{(+)}_{\mathrm{R21}}\rho^{(n)}_{\mathrm{QS},00}\right]$$

$$+\,\mathrm{H.c.},\tag{I.38-2}$$

$$\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}(t)\big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\big|_{05,\mathrm{con}}\Big|_{04}|0\rangle\Big|_{03}$$

$$=-a_+a_+b_+b_+\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}$$

$$\times\Big[C^{(-)}_{\mathrm{L03}}C^{(-)}_{\mathrm{L21}}\rho^{(n)}_{\mathrm{QS},11,11}+C^{(-)}_{\mathrm{L03}}C^{(-)}_{\mathrm{R21}}\rho^{(n-1)}_{\mathrm{QS},11,11}+C^{(-)}_{\mathrm{R03}}C^{(-)}_{\mathrm{L21}}\rho^{(n-1)}_{\mathrm{QS},11,11}+C^{(-)}_{\mathrm{R03}}C^{(-)}_{\mathrm{R21}}\rho^{(n-2)}_{\mathrm{QS},11,11}\Big]$$

$$
\begin{aligned}
&-a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_+t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}\\
&\times\Big[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\Big]\\
&+\mathrm{H.c.},
\end{aligned}
\tag{I.38-3}
$$

$$
\begin{aligned}
&\langle 0|\mathrm{e}^{-\mathrm{i}H_{\mathrm{QS}}t}\rho_{\mathrm{QS,I}}\left(t\right)\Big|_{\text{fourth-order}}\mathrm{e}^{\mathrm{i}H_{\mathrm{QS}}t}\Big|_{05,\mathrm{con}}\Big|_{04}|0\rangle\Big|_{04}\\
=&-a_+a_-b_+b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_+)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_+t_3}\\
&\times\Big[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\Big]\\
&-a_-a_-b_-b_-\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\mathrm{i}\varepsilon_-t}\mathrm{e}^{-\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_1}\mathrm{e}^{\mathrm{i}(\varepsilon_{1,1}-\varepsilon_-)t_2}\mathrm{e}^{-\mathrm{i}\varepsilon_-t_3}\\
&\times\Big[C_{\mathrm{L03}}^{(-)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n)}+C_{\mathrm{L03}}^{(-)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{L21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-1)}+C_{\mathrm{R03}}^{(-)}C_{\mathrm{R21}}^{(-)}\rho_{\mathrm{QS},11,11}^{(n-2)}\Big]\\
&+\mathrm{H.c.}.
\end{aligned}
\tag{I.38-4}
$$

# 附录 J　共隧穿过程中的 16 类积分

在本附录中，给出在共隧穿极限下计算开放量子系统约化密度矩阵运动方程时，用到的 16 个积分. 此外，在下面的推导中，令 $\hbar\equiv 1$. 由式 (4.9) 可知

$$a_{\alpha\mu}^{\dagger}\left(t\right)=\sum\nolimits_{\alpha\boldsymbol{k}\sigma}t_{\alpha\mu\boldsymbol{k}\sigma}\mathrm{e}^{\mathrm{i}H_{\mathrm{leads}}t}a_{\alpha\boldsymbol{k}\sigma}^{\dagger}\mathrm{e}^{-\mathrm{i}H_{\mathrm{leads}}t},\tag{J.1}$$

$$a_{\alpha\mu}\left(t\right)=\sum\nolimits_{\alpha\boldsymbol{k}\sigma}t_{\alpha\mu\boldsymbol{k}\sigma}^{*}\mathrm{e}^{\mathrm{i}H_{\mathrm{leads}}t}a_{\alpha\boldsymbol{k}\sigma}\mathrm{e}^{-\mathrm{i}H_{\mathrm{leads}}t},\tag{J.2}$$

由于

$$\mathrm{e}^{\mathrm{i}H_{\mathrm{leads}}t}a_{\alpha\boldsymbol{k}\sigma}^{\dagger}\mathrm{e}^{-\mathrm{i}H_{\mathrm{leads}}t}=\mathrm{e}^{\mathrm{i}\varepsilon_{\alpha\boldsymbol{k}\sigma}t}a_{\alpha\boldsymbol{k}\sigma}^{\dagger},\tag{J.3}$$

$$\mathrm{e}^{\mathrm{i}H_{\mathrm{leads}}t}a_{\alpha\boldsymbol{k}\sigma}\mathrm{e}^{-\mathrm{i}H_{\mathrm{leads}}t}=\mathrm{e}^{-\mathrm{i}\varepsilon_{\alpha\boldsymbol{k}\sigma}t}a_{\alpha\boldsymbol{k}\sigma},\tag{J.4}$$

将式 (J.3) 和式 (J.4) 分别代入式 (J.1) 和式 (J.2) 可得

$$a_{\alpha\mu}^{\dagger}\left(t\right)=\sum\nolimits_{\alpha\boldsymbol{k}\sigma}t_{\alpha\mu\boldsymbol{k}\sigma}\mathrm{e}^{\mathrm{i}\varepsilon_{\alpha\boldsymbol{k}\sigma}t}a_{\alpha\boldsymbol{k}\sigma}^{\dagger},\tag{J.5}$$

$$a_{\alpha\mu}\left(t\right)=\sum\nolimits_{\alpha\boldsymbol{k}\sigma}t_{\alpha\mu\boldsymbol{k}\sigma}^{*}\mathrm{e}^{-\mathrm{i}\varepsilon_{\alpha\boldsymbol{k}\sigma}t}a_{\alpha\boldsymbol{k}\sigma}.\tag{J.6}$$

需要说明的是，为了避免电极产生和湮灭算符中的波矢量与电子库谱函数中的记号 $k$ 混淆，在式 (J.3)~(J.6) 中，将电极产生和湮灭算符中的波矢量记为 $\boldsymbol{k}$. 若电极的态密度选择洛伦兹截断，即

$$\rho_{\alpha\sigma}\left(\varepsilon\right)=\rho_{\alpha\sigma}g_{\alpha}\left(\varepsilon\right)=\rho_{\alpha\sigma}\frac{W^2}{\left(\varepsilon-\mu_{\alpha}\right)^2+W^2},\tag{J.7}$$

并定义隧穿概率 $\Gamma_{\alpha\sigma}^{\mu\mu'}$

$$\Gamma_{\alpha\sigma}^{\mu\mu'}=\sum_{\alpha\mu\mu'\sigma}2\pi\rho_{\alpha\sigma}\left|t_{\alpha\sigma}^{\mu\mu'}\right|^{2}, \tag{J.8}$$

则电极的谱函数可以表示为

$$C_{\alpha02}^{(+)}=\frac{\Gamma_{\alpha\sigma}^{ik}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega g_{\alpha}\left(\omega\right)\mathrm{e}^{\mathrm{i}\omega(t-t_{2})}f_{\alpha}^{(+)}\left(\omega\right), \tag{J.9}$$

$$C_{\alpha02}^{(-)}=\frac{\Gamma_{\alpha\sigma}^{ik}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega g_{\alpha}\left(\omega\right)\mathrm{e}^{-\mathrm{i}\omega(t-t_{2})}f_{\alpha}^{(-)}\left(\omega\right), \tag{J.10}$$

$$C_{\alpha13}^{(+)}=\frac{\Gamma_{\alpha\sigma}^{jl}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega g_{\alpha}\left(\omega\right)\mathrm{e}^{\mathrm{i}\omega(t_{1}-t_{3})}f_{\alpha}^{(+)}\left(\omega\right), \tag{J.11}$$

$$C_{\alpha13}^{(-)}=\frac{\Gamma_{\alpha\sigma}^{jl}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega g_{\alpha}\left(\omega\right)\mathrm{e}^{-\mathrm{i}\omega(t_{1}-t_{3})}f_{\alpha}^{(-)}\left(\omega\right), \tag{J.12}$$

$$C_{\alpha31}^{(+)}=\frac{\Gamma_{\alpha\sigma}^{lj}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega g_{\alpha}\left(\omega\right)\mathrm{e}^{\mathrm{i}\omega(t_{3}-t_{1})}f_{\alpha}^{(+)}\left(\omega\right), \tag{J.13}$$

$$C_{\alpha31}^{(-)}=\frac{\Gamma_{\alpha\sigma}^{lj}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega g_{\alpha}\left(\omega\right)\mathrm{e}^{-\mathrm{i}\omega(t_{3}-t_{1})}f_{\alpha}^{(-)}\left(\omega\right), \tag{J.14}$$

$$C_{\alpha03}^{(+)}=\frac{\Gamma_{\alpha\sigma}^{il}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega g_{\alpha}\left(\omega\right)\mathrm{e}^{\mathrm{i}\omega(t-t_{3})}f_{\alpha}^{(+)}\left(\omega\right), \tag{J.15}$$

$$C_{\alpha03}^{(-)}=\frac{\Gamma_{\alpha\sigma}^{il}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega g_{\alpha}\left(\omega\right)\mathrm{e}^{-\mathrm{i}\omega(t-t_{3})}f_{\alpha}^{(-)}\left(\omega\right), \tag{J.16}$$

$$C_{\alpha12}^{(+)}=\frac{\Gamma_{\alpha\sigma}^{jk}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega g_{\alpha}\left(\omega\right)\mathrm{e}^{\mathrm{i}\omega(t_{1}-t_{2})}f_{\alpha}^{(+)}\left(\omega\right), \tag{J.17}$$

$$C_{\alpha12}^{(-)}=\frac{\Gamma_{\alpha\sigma}^{jk}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega g_{\alpha}\left(\omega\right)\mathrm{e}^{-\mathrm{i}\omega(t_{1}-t_{2})}f_{\alpha}^{(-)}\left(\omega\right), \tag{J.18}$$

$$C_{\alpha21}^{(+)}=\frac{\Gamma_{\alpha\sigma}^{kj}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega g_{\alpha}\left(\omega\right)\mathrm{e}^{\mathrm{i}\omega(t_{2}-t_{1})}f_{\alpha}^{(+)}\left(\omega\right), \tag{J.19}$$

$$C_{\alpha21}^{(-)}=\frac{\Gamma_{\alpha\sigma}^{kj}}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}\omega g_{\alpha}\left(\omega\right)\mathrm{e}^{-\mathrm{i}\omega(t_{2}-t_{1})}f_{\alpha}^{(-)}\left(\omega\right). \tag{J.20}$$

在共隧穿极限下，若将相关的系数忽略，开放量子系统约化密度矩阵运动方程涉及的矩阵元形式上有如下 8 种类型：

$$C_{\alpha02}^{(\pm)}C_{\alpha'13}^{(\pm)}\int_{t_{0}}^{t}\mathrm{d}t_{1}\int_{t_{0}}^{t_{1}}\mathrm{d}t_{2}\int_{t_{0}}^{t_{2}}\mathrm{d}t_{3}\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_{1}}\mathrm{e}^{\mathrm{i}bt_{2}}\mathrm{e}^{\mathrm{i}ct_{3}}, \tag{J.21}$$

$$C_{\alpha02}^{(\pm)}C_{\alpha'13}^{(\mp)}\int_{t_{0}}^{t}\mathrm{d}t_{1}\int_{t_{0}}^{t_{1}}\mathrm{d}t_{2}\int_{t_{0}}^{t_{2}}\mathrm{d}t_{3}\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_{1}}\mathrm{e}^{\mathrm{i}bt_{2}}\mathrm{e}^{\mathrm{i}ct_{3}}, \tag{J.22}$$

$$C_{\alpha 02}^{(\pm)}C_{\alpha' 31}^{(\pm)}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3},\tag{J.23}$$

$$C_{\alpha 02}^{(\pm)}C_{\alpha' 31}^{(\mp)}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3},\tag{J.24}$$

$$C_{\alpha 03}^{(\pm)}C_{\alpha' 12}^{(\pm)}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3},\tag{J.25}$$

$$C_{\alpha 03}^{(\pm)}C_{\alpha' 12}^{(\mp)}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3},\tag{J.26}$$

$$C_{\alpha 03}^{(\pm)}C_{\alpha' 21}^{(\pm)}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3},\tag{J.27}$$

$$C_{\alpha 03}^{(\pm)}C_{\alpha' 21}^{(\mp)}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3},\tag{J.28}$$

其中，系数 $a$，$b$ 和 $c$ 依赖于矩阵元. 对于式 (2.17) 描述的微扰项缓慢打开的情形，选取 $\eta\to 0^+$，此时 $t_0\to-\infty$，式 (J.21) 中的积分下限可以改写为

$$C_{\alpha 02}^{(\pm)}C_{\alpha' 13}^{(\pm)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3},\tag{J.29}$$

将式 (J.9)~ 式 (J.12) 代入上式可得

$$\begin{aligned}
&C_{\alpha 02}^{(\pm)}C_{\alpha' 13}^{(\pm)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\\
=&\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\lim_{\eta\to 0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\pm)}(\omega_2)\\
&\times\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\pm\mathrm{i}\omega_1(t-t_2)}\mathrm{e}^{\pm\mathrm{i}\omega_2(t_1-t_3)}\\
&\times\mathrm{e}^{-\mathrm{i}(a+b+c+\mathrm{i}\eta)t}\mathrm{e}^{\mathrm{i}(a-\mathrm{i}\eta)t_1}\mathrm{e}^{\mathrm{i}(b-\mathrm{i}\eta)t_2}\mathrm{e}^{\mathrm{i}(c-\mathrm{i}\eta)t_3}\\
=&\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\lim_{\eta\to 0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\pm)}(\omega_2)\\
&\times\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\pm\mathrm{i}[\omega_1\mp(a+b+c)\mp\mathrm{i}\eta]t}\\
&\times\mathrm{e}^{\pm\mathrm{i}(\omega_2\pm a\mp\mathrm{i}\eta)t_1}\mathrm{e}^{\mp\mathrm{i}(\omega_1\mp b\pm\mathrm{i}\eta)t_2}\mathrm{e}^{\mp\mathrm{i}(\omega_2\mp c\pm\mathrm{i}\eta)t_3},
\end{aligned}\tag{J.30}$$

对式 (J.30) 求关于时间 $t_1$，$t_2$ 和 $t_3$ 的积分可得

$$
\begin{aligned}
&C_{\alpha 02}^{(\pm)}C_{\alpha' 13}^{(\pm)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\\
=&\frac{-\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\pm)}(\omega_2)\\
&\times\frac{1}{a+c}\left(\frac{1}{\omega_1\mp a\mp b\mp c\pm\mathrm{i}\eta}\frac{1}{\omega_1+\omega_2\mp a\mp b\mp 2c\pm\mathrm{i}\eta}\right.\\
&-\frac{1}{\omega_1\mp a\mp b\mp c\pm\mathrm{i}\eta}\frac{1}{\omega_1+\omega_2\mp b\mp c\pm\mathrm{i}\eta}\\
&+\frac{1}{\omega_2\mp c\pm\mathrm{i}\eta}\frac{1}{\omega_1+\omega_2\mp a\mp b\mp 2c\pm\mathrm{i}\eta}\\
&\left.-\frac{1}{\omega_2\mp c\pm\mathrm{i}\eta}\frac{1}{\omega_1+\omega_2\mp b\mp c\pm\mathrm{i}\eta}\right),
\end{aligned}
\tag{J.31}
$$

式 (J.31) 通常情况下为复数，其实部可表示为

$$
\begin{aligned}
&C_{\alpha 02}^{(\pm)}C_{\alpha' 13}^{(\pm)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\Big|_{\mathrm{Re}}\\
=&\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\pm)}(\omega_2)\\
&\times\frac{1}{a+c}\mathrm{Im}\left(\frac{1}{\omega_1\mp a\mp b\mp c\pm\mathrm{i}\eta}\frac{1}{\omega_1+\omega_2\mp a\mp b\mp 2c\pm\mathrm{i}\eta}\right.\\
&-\frac{1}{\omega_1\mp a\mp b\mp c\pm\mathrm{i}\eta}\frac{1}{\omega_1+\omega_2\mp b\mp c\pm\mathrm{i}\eta}\\
&+\frac{1}{\omega_2\mp c\pm\mathrm{i}\eta}\frac{1}{\omega_1+\omega_2\mp a\mp b\mp 2c\pm\mathrm{i}\eta}\\
&\left.-\frac{1}{\omega_2\mp c\pm\mathrm{i}\eta}\frac{1}{\omega_1+\omega_2\mp b\mp c\pm\mathrm{i}\eta}\right),
\end{aligned}
\tag{J.32}
$$

利用 $\delta$ 函数的性质

$$
\lim_{\eta\to0^+}\frac{\eta}{x^2+\eta^2}=\pi\delta(x),
\tag{J.33}
$$

将式 (J.32) 进一步展开可得

$$
\begin{aligned}
&C_{\alpha 02}^{(\pm)}C_{\alpha' 13}^{(\pm)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\Big|_{\mathrm{Re}}\\
=&\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\pm)}(\omega_2)\\
&\times\frac{\mp\pi}{a+c}P\left(\frac{\delta(\omega_1\mp a\mp b\mp c)}{\omega_1+\omega_2\mp a\mp b\mp 2c}+\frac{\delta(\omega_1+\omega_2\mp a\mp b\mp 2c)}{\omega_1\mp a\mp b\mp c}\right.
\end{aligned}
$$

$$
-\frac{\delta\left(\omega_1\mp a\mp b\mp c\right)}{\omega_1+\omega_2\mp b\mp c}-\frac{\delta\left(\omega_1+\omega_2\mp b\mp c\right)}{\omega_1\mp a\mp b\mp c}
$$

$$
+\frac{\delta\left(\omega_2\mp c\right)}{\omega_1+\omega_2\mp a\mp b\mp 2c}+\frac{\delta\left(\omega_1+\omega_2\mp a\mp b\mp 2c\right)}{\omega_2\mp c}
$$

$$
\left.-\frac{\delta\left(\omega_2\mp c\right)}{\omega_1+\omega_2\mp b\mp c}-\frac{\delta\left(\omega_1+\omega_2\mp b\mp c\right)}{\omega_2\mp c}\right), \tag{J.34}
$$

将式 (J.34) 进一步简化为

$$
\begin{aligned}
&C_{\alpha 02}^{(\pm)}C_{\alpha' 13}^{(\pm)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\Big|_{\mathrm{Re}}\\
=&\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\mp\pi}{a+c}f_{\alpha}^{(\pm)}\left(\pm a\pm b\pm c\right)P\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}\left(\omega_2\right)f_{\alpha'}^{(\pm)}\left(\omega_2\right)\frac{1}{\omega_2\mp c}\\
&-\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\mp\pi}{a+c}f_{\alpha}^{(\pm)}\left(\pm a\pm b\pm c\right)P\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}\left(\omega_2\right)f_{\alpha'}^{(\pm)}\left(\omega_2\right)\frac{1}{\omega_2\pm a}\\
&+\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\mp\pi}{a+c}f_{\alpha'}^{(\pm)}\left(\pm c\right)P\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_{\alpha}\left(\omega_1\right)f_{\alpha}^{(\pm)}\left(\omega_1\right)\frac{1}{\omega_1\mp a\mp b\mp c}\\
&-\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\mp\pi}{a+c}f_{\alpha'}^{(\pm)}\left(\pm c\right)P\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_{\alpha}\left(\omega_1\right)f_{\alpha}^{(\pm)}\left(\omega_1\right)\frac{1}{\omega_1\mp b}\\
&-\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\pm\pi}{a+c}P\int_{-\infty}^{\infty}\mathrm{d}\omega_2 f_{\alpha}^{(\pm)}\left(-\omega_2\pm b\pm c\right)g_{\alpha'}\left(\omega_2\right)f_{\alpha'}^{(\pm)}\left(\omega_2\right)\frac{1}{\omega_2\pm a}\\
&-\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\mp\pi}{a+c}P\int_{-\infty}^{\infty}\mathrm{d}\omega_2 f_{\alpha}^{(\pm)}\left(-\omega_2\pm b\pm c\right)g_{\alpha'}\left(\omega_2\right)f_{\alpha'}^{(\pm)}\left(\omega_2\right)\frac{1}{\omega_2\mp c},
\end{aligned} \tag{J.35}
$$

其中，$P$ 为主值积分. 此外，上式推导中利用了宽带近似. 同理，式 (J.31) 的虚部表示为

$$
\begin{aligned}
&C_{\alpha 02}^{(\pm)}C_{\alpha' 13}^{(\pm)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\Big|_{\mathrm{Im}}\\
=&\frac{-\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\lim_{\eta\to 0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_{\alpha}\left(\omega_1\right)f_{\alpha}^{(\pm)}\left(\omega_1\right)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}\left(\omega_2\right)f_{\alpha'}^{(\pm)}\left(\omega_2\right)\\
&\times\frac{1}{a+c}\mathrm{Re}\left(\frac{1}{\omega_1\mp a\mp b\mp c\pm\mathrm{i}\eta}\frac{1}{\omega_1+\omega_2\mp a\mp b\mp 2c\pm\mathrm{i}\eta}\right.\\
&-\frac{1}{\omega_1\mp a\mp b\mp c\pm\mathrm{i}\eta}\frac{1}{\omega_1+\omega_2\mp b\mp c\pm\mathrm{i}\eta}\\
&+\frac{1}{\omega_2\mp c\pm\mathrm{i}\eta}\frac{1}{\omega_1+\omega_2\mp a\mp b\mp 2c\pm\mathrm{i}\eta}
\end{aligned}
$$

$$
-\frac{1}{\omega_2\mp c\pm \mathrm{i}\eta}\frac{1}{\omega_1+\omega_2\mp b\mp c\pm \mathrm{i}\eta}\bigg), \tag{J.36}
$$

利用式 (J.33) 描述的 $\delta$ 函数性质，可将式 (J.36) 进一步简化为

$$
\begin{aligned}
&C_{\alpha 02}^{(\pm)}C_{\alpha' 13}^{(\pm)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\bigg|_{\mathrm{Im}}\\
=&\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\lim_{\eta\to 0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\pm)}(\omega_2)\\
&\times\frac{\pi^2}{a+c}\Big(\delta(\omega_1\mp a\mp b\mp c)\,\delta(\omega_1+\omega_2\mp a\mp b\mp 2c)\\
&-\delta(\omega_1\mp a\mp b\mp c)\,\delta(\omega_1+\omega_2\mp b\mp c)\\
&+\delta(\omega_2\mp c)\,\delta(\omega_1+\omega_2\mp a\mp b\mp 2c)-\delta(\omega_2\mp c)\,\delta(\omega_1+\omega_2\mp b\mp c)\\
&+\frac{1}{\omega_1\mp a\mp b\mp c}\frac{1}{\omega_1+\omega_2\mp a\mp b\mp 2c}-\frac{1}{\omega_1\mp a\mp b\mp c}\frac{1}{\omega_1+\omega_2\mp b\mp c}\\
&+\frac{1}{\omega_2\mp c}\frac{1}{\omega_1+\omega_2\mp a\mp b\mp 2c}-\frac{1}{\omega_2\mp c}\frac{1}{\omega_1+\omega_2\mp b\mp c}\Big],
\end{aligned} \tag{J.37}
$$

将式 (J.37) 进一步整理可得

$$
\begin{aligned}
&C_{\alpha 02}^{(\pm)}C_{\alpha' 13}^{(\pm)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\bigg|_{\mathrm{Im}}\\
=&\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\pi^2}{a+c}\Big[2f_\alpha^{(\pm)}(\pm a\pm b\pm c)\,f_{\alpha'}^{(\pm)}(\pm c)\\
&-f_\alpha^{(\pm)}(\pm a\pm b\pm c)\,f_{\alpha'}^{(\pm)}(\mp a)-f_\alpha^{(\pm)}(\pm b)\,f_{\alpha'}^{(\pm)}(\pm c)\Big]\\
&-\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\pm)}(\omega_2)\\
&\times\frac{1}{\omega_1\mp a\mp b\mp c}\frac{1}{\omega_2\mp c}\frac{1}{\omega_1+\omega_2\mp b\mp c}.
\end{aligned} \tag{J.38}
$$

同理，式 (J.22) 可表示为

$$
\begin{aligned}
&C_{\alpha 02}^{(\pm)}C_{\alpha' 13}^{(\mp)}\int_{t_0}^{t}\mathrm{d}t_1\int_{t_0}^{t_1}\mathrm{d}t_2\int_{t_0}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\\
=&\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\lim_{\eta\to 0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\pm\mathrm{i}\omega_1(t-t_2)}\mathrm{e}^{\mp\mathrm{i}\omega_2(t_1-t_3)}\\
&\times\mathrm{e}^{-\mathrm{i}(a+b+c+\mathrm{i}\eta)t}\mathrm{e}^{\mathrm{i}(a-\mathrm{i}\eta)t_1}\mathrm{e}^{\mathrm{i}(b-\mathrm{i}\eta)t_2}\mathrm{e}^{\mathrm{i}(c-\mathrm{i}\eta)t_3}\\
=&\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\lim_{\eta\to 0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\mp)}(\omega_2)
\end{aligned}
$$

$$
\begin{aligned}
&\times \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{\pm\mathrm{i}[\omega_1 \mp (a+b+c) \mp \mathrm{i}\eta]t} \\
&\times \mathrm{e}^{\mp\mathrm{i}(\omega_2 \mp a \pm \mathrm{i}\eta)t_1} \mathrm{e}^{\mp\mathrm{i}(\omega_1 \mp b \pm \mathrm{i}\eta)t_2} \mathrm{e}^{\pm\mathrm{i}(\omega_2 \pm c \mp \mathrm{i}\eta)t_3},
\end{aligned} \tag{J.39}
$$

对式 (J.39) 求关于时间 $t_1$，$t_2$ 和 $t_3$ 的积分可得

$$
\begin{aligned}
&C^{(\pm)}_{\alpha 02} C^{(\mp)}_{\alpha' 13} \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{-\mathrm{i}(a+b+c)t} \mathrm{e}^{\mathrm{i}at_1} \mathrm{e}^{\mathrm{i}bt_2} \mathrm{e}^{\mathrm{i}ct_3} \\
=& \frac{\pm\mathrm{i}\Gamma^{ik}_{\alpha\sigma}\Gamma^{jl}_{\alpha'\sigma}}{(2\pi)^2} \lim_{\eta\to 0^+} \int_{-\infty}^{\infty} \mathrm{d}\omega_1 g_{\alpha}(\omega_1) f^{(\pm)}_{\alpha}(\omega_1) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f^{(\mp)}_{\alpha'}(\omega_2) \\
&\times \frac{1}{(\omega_1 \mp a \mp c \mp b \pm \mathrm{i}\eta)(\omega_2 \pm c \mp \mathrm{i}\eta)(\omega_1 - \omega_2 \mp c \mp b \pm \mathrm{i}\eta)} \\
=& \frac{\mathrm{i}\Gamma^{ik}_{\alpha\sigma}\Gamma^{jl}_{\alpha'\sigma}}{(2\pi)^2} \lim_{\eta\to 0^+} \int_{-\infty}^{\infty} \mathrm{d}\omega_1 g_{\alpha}(\omega_1) f^{(\pm)}_{\alpha}(\omega_1) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f^{(\mp)}_{\alpha'}(\omega_2) \\
&\times \frac{1}{a+c} \left( \frac{1}{\omega_2 \pm c \mp \mathrm{i}\eta} \frac{1}{\omega_1 - \omega_2 \mp a \mp 2c \mp b \pm \mathrm{i}\eta} \right. \\
&- \frac{1}{\omega_2 \pm c \mp \mathrm{i}\eta} \frac{1}{\omega_1 - \omega_2 \mp c \mp b \pm \mathrm{i}\eta} \\
&- \frac{1}{\omega_1 \mp a \mp c \mp b \pm \mathrm{i}\eta} \frac{1}{\omega_1 - \omega_2 \mp a \mp 2c \mp b \pm \mathrm{i}\eta} \\
&\left. + \frac{1}{\omega_1 \mp a \mp c \mp b \pm \mathrm{i}\eta} \frac{1}{\omega_1 - \omega_2 \mp c \mp b \pm \mathrm{i}\eta} \right),
\end{aligned} \tag{J.40}
$$

利用式 (J.33) 描述的 $\delta$ 函数性质，式 (J.40) 的实部可表示为

$$
\begin{aligned}
&C^{(\pm)}_{\alpha 02} C^{(\mp)}_{\alpha' 13} \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{-\mathrm{i}(a+b+c)t} \mathrm{e}^{\mathrm{i}at_1} \mathrm{e}^{\mathrm{i}bt_2} \mathrm{e}^{\mathrm{i}ct_3} \Big|_{\mathrm{Re}} \\
=& \frac{\Gamma^{ik}_{\alpha\sigma}\Gamma^{jl}_{\alpha'\sigma}}{(2\pi)^2} \frac{\mp\pi}{a+c} \int_{-\infty}^{\infty} \mathrm{d}\omega_1 g_{\alpha}(\omega_1) f^{(\pm)}_{\alpha}(\omega_1) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f^{(\mp)}_{\alpha'}(\omega_2) \\
&\times \left[ \frac{\delta(\omega_2 \pm c)}{\omega_1 - \omega_2 \mp a \mp 2c \mp b} - \frac{\delta(\omega_1 - \omega_2 \mp a \mp 2c \mp b)}{\omega_2 \pm c} \right. \\
&- \frac{\delta(\omega_2 \pm c)}{\omega_1 - \omega_2 \mp c \mp b} + \frac{\delta(\omega_1 - \omega_2 \mp c \mp b)}{\omega_2 \pm c} \\
&+ \frac{\delta(\omega_1 \mp a \mp c \mp b)}{\omega_1 - \omega_2 \mp a \mp 2c \mp b} + \frac{\delta(\omega_1 - \omega_2 \mp a \mp 2c \mp b)}{\omega_1 \mp a \mp c \mp b} \\
&\left. - \frac{\delta(\omega_1 \mp a \mp c \mp b)}{\omega_1 - \omega_2 \mp c \mp b} - \frac{\delta(\omega_1 - \omega_2 \mp c \mp b)}{\omega_1 \mp a \mp c \mp b} \right],
\end{aligned} \tag{J.41}
$$

式 (J.41) 可进一步整理为

$$\begin{aligned}
&C_{\alpha 02}^{(\pm)}C_{\alpha' 13}^{(\mp)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\Big|_{\mathrm{Re}}\\
=&\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\pm\pi}{a+c}f_{\alpha}^{(\pm)}(\pm a\pm c\pm b)P\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\mp)}(\omega_2)\frac{1}{\omega_2\pm c}\\
&-\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\pm\pi}{a+c}f_{\alpha}^{(\pm)}(\pm a\pm c\pm b)P\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\mp)}(\omega_2)\frac{1}{\omega_2\mp a}\\
&+\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\mp\pi}{a+c}f_{\alpha'}^{(\mp)}(\mp c)P\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_{\alpha}(\omega_1)f_{\alpha}^{(\pm)}(\omega_1)\frac{1}{\omega_1\mp a\mp c\mp b}\\
&-\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\mp\pi}{a+c}f_{\alpha'}^{(\mp)}(\mp c)P\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_{\alpha}(\omega_1)f_{\alpha}^{(\pm)}(\omega_1)\frac{1}{\omega_1\mp b}\\
&+\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\mp\pi}{a+c}P\int_{-\infty}^{\infty}\mathrm{d}\omega_2 f_{\alpha}^{(\pm)}(\omega_2\pm c\pm b)g_{\alpha'}(\omega_2)f_{\alpha'}^{(\mp)}(\omega_2)\frac{1}{\omega_2\pm c}\\
&-\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\mp\pi}{a+c}P\int_{-\infty}^{\infty}\mathrm{d}\omega_2 f_{\alpha}^{(\pm)}(\omega_2\pm b\pm c)g_{\alpha'}(\omega_2)f_{\alpha'}^{(\mp)}(\omega_2)\frac{1}{\omega_2\mp a},
\end{aligned}\tag{J.42}$$

由式 (J.40) 可知，其虚部可表示为

$$\begin{aligned}
&C_{\alpha 02}^{(\pm)}C_{\alpha' 13}^{(\mp)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\Big|_{\mathrm{Im}}\\
=&\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\pi^2}{a+c}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_{\alpha}(\omega_1)f_{\alpha}^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times[\delta(\omega_2\pm c)\delta(\omega_1-\omega_2\mp a\mp 2c\mp b)-\delta(\omega_2\pm c)\delta(\omega_1-\omega_2\mp c\mp b)\\
&+\delta(\omega_1\mp a\mp c\mp b)\delta(\omega_1-\omega_2\mp a\mp 2c\mp b)\\
&-\delta(\omega_1\mp a\mp c\mp b)\delta(\omega_1-\omega_2\mp c\mp b)]\\
&\pm\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{1}{a+c}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_{\alpha}(\omega_1)f_{\alpha}^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times\frac{1}{\omega_1\mp a\mp c\mp b}\frac{1}{\omega_2\pm c}\frac{1}{\omega_1-\omega_2\mp c\mp b},
\end{aligned}\tag{J.43}$$

式 (J.43) 可进一步整理为

$$C_{\alpha 02}^{(\pm)}C_{\alpha' 13}^{(\mp)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\Big|_{\mathrm{Im}}$$

$$
\begin{aligned}
&=\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\pi^2}{a+c}\Big[2f_{\alpha}^{(\pm)}(\pm a\pm c\pm b)f_{\alpha'}^{(\mp)}(\mp c)\\
&-f_{\alpha}^{(\pm)}(\pm a\pm c\pm b)f_{\alpha'}^{(\mp)}(\pm a)-f_{\alpha}^{(\pm)}(\pm b)f_{\alpha'}^{(\mp)}(\mp c)\Big]\\
&\pm\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times\frac{1}{\omega_1\mp a\mp c\mp b}\frac{1}{\omega_2\pm c}\frac{1}{\omega_1-\omega_2\mp c\mp b}.
\end{aligned}\tag{J.44}
$$

对式 (J.23) 求关于时间 $t_1$，$t_2$ 和 $t_3$ 的积分可得

$$
\begin{aligned}
&C_{\alpha 02}^{(\pm)}C_{\alpha'31}^{(\pm)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\\
=&\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\pm)}(\omega_2)\\
&\times\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\pm\mathrm{i}\omega_1(t-t_2)}\mathrm{e}^{\pm\mathrm{i}\omega_2(t_3-t_1)}\\
&\times\mathrm{e}^{-\mathrm{i}(a+b+c+\mathrm{i}\eta)t}\mathrm{e}^{\mathrm{i}(a-\mathrm{i}\eta)t_1}\mathrm{e}^{\mathrm{i}(b-\mathrm{i}\eta)t_2}\mathrm{e}^{\mathrm{i}(c-\mathrm{i}\eta)t_3}\\
=&\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\pm)}(\omega_2)\\
&\times\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\pm\mathrm{i}[\omega_1\mp(a+b+c)\mp\mathrm{i}\eta]t}\\
&\times\mathrm{e}^{\mp\mathrm{i}(\omega_2\mp a\pm\mathrm{i}\eta)t_1}\mathrm{e}^{\mp\mathrm{i}(\omega_1\mp b\pm\mathrm{i}\eta)t_2}\mathrm{e}^{\pm\mathrm{i}(\omega_2\pm c\mp\mathrm{i}\eta)t_3}\\
=&\frac{\pm\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)g_{\alpha'}(\omega_2)f_{\alpha'}^{(\pm)}(\omega_2)\\
&\times\frac{1}{(\omega_1\mp a\mp c\mp b\pm\mathrm{i}\eta)(\omega_2\pm c\mp\mathrm{i}\eta)(\omega_1-\omega_2\mp c\mp b\pm\mathrm{i}\eta)}\\
=&\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\frac{1}{a+c}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)g_{\alpha'}(\omega_2)f_{\alpha'}^{(\pm)}(\omega_2)\\
&\times\bigg(\frac{1}{\omega_2\pm c\mp\mathrm{i}\eta}\frac{1}{\omega_1-\omega_2\mp a\mp 2c\mp b\pm\mathrm{i}\eta}-\frac{1}{\omega_2\pm c\mp\mathrm{i}\eta}\frac{1}{\omega_1-\omega_2\mp c\mp b\pm\mathrm{i}\eta}\\
&-\frac{1}{\omega_1\mp a\mp c\mp b\pm\mathrm{i}\eta}\frac{1}{\omega_1-\omega_2\mp a\mp 2c\mp b\pm\mathrm{i}\eta}\\
&+\frac{1}{\omega_1\mp a\mp c\mp b\pm\mathrm{i}\eta}\frac{1}{\omega_1-\omega_2\mp c\mp b\pm\mathrm{i}\eta}\bigg),
\end{aligned}\tag{J.45}
$$

式 (J.45) 的实部可表示为

$$
C_{\alpha 02}^{(\pm)}C_{\alpha'31}^{(\pm)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\bigg|_{\mathrm{Re}}
$$

$$
\begin{aligned}
=&\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\frac{\pm\pi}{a+c}f_{\alpha}^{(\pm)}(\pm a\pm c\pm b)\,P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)\,f_{\alpha'}^{(\pm)}(\omega_2)}{\omega_2\pm c}\\
&-\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\frac{\pm\pi}{a+c}f_{\alpha}^{(\pm)}(\pm a\pm c\pm b)\,P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)\,f_{\alpha'}^{(\pm)}(\omega_2)}{\omega_2\mp a}\\
&+\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\frac{\mp\pi}{a+c}f_{\alpha'}^{(\pm)}(\mp c)\,P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\frac{g_{\alpha}(\omega_1)\,f_{\alpha}^{(\pm)}(\omega_1)}{\omega_1\mp a\mp c\mp b}\\
&-\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\frac{\mp\pi}{a+c}f_{\alpha'}^{(\pm)}(\mp c)\,P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\frac{g_{\alpha}(\omega_1)\,f_{\alpha}^{(\pm)}(\omega_1)}{\omega_1\mp b}\\
&+\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\mp\pi}{a+c}P\int_{-\infty}^{\infty}\mathrm{d}\omega_2 f_{\alpha}^{(\pm)}(\omega_2\pm c\pm b)\,g_{\alpha'}(\omega_2)\,f_{\alpha'}^{(\pm)}(\omega_2)\,\frac{1}{\omega_2\pm c}\\
&-\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\mp\pi}{a+c}P\int_{-\infty}^{\infty}\mathrm{d}\omega_2 f_{\alpha}^{(\pm)}(\omega_2\pm b\pm c)\,g_{\alpha'}(\omega_2)\,f_{\alpha'}^{(\pm)}(\omega_2)\,\frac{1}{\omega_2\mp a},
\end{aligned}\tag{J.46}
$$

同理，式 (J.45) 的虚部可表示为

$$
\begin{aligned}
&C_{\alpha02}^{(\pm)}C_{\alpha'31}^{(\pm)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\Big|_{\mathrm{Im}}\\
=&\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\frac{\pi^2}{a+c}\Big[2f_{\alpha}^{(\pm)}(\pm a\pm c\pm b)\,f_{\alpha'}^{(\pm)}(\mp c)\\
&-f_{\alpha}^{(\pm)}(\pm a\pm c\pm b)\,f_{\alpha'}^{(\pm)}(\pm a)-f_{\alpha}^{(\pm)}(\pm b)\,f_{\alpha'}^{(\pm)}(\mp c)\Big]\\
&\pm\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_{\alpha}(\omega_1)\,f_{\alpha}^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)\,f_{\alpha'}^{(\pm)}(\omega_2)\\
&\times\frac{1}{\omega_1\mp a\mp c\mp b}\frac{1}{\omega_2\pm c}\frac{1}{\omega_1-\omega_2\mp c\mp b},
\end{aligned}\tag{J.47}
$$

对式 (J.24) 求关于时间 $t_1$，$t_2$ 和 $t_3$ 的积分可得

$$
\begin{aligned}
&C_{\alpha02}^{(\pm)}C_{\alpha'31}^{(\mp)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\\
=&\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_{\alpha}(\omega_1)\,f_{\alpha}^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)\,f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\pm\mathrm{i}\omega_1(t-t_2)}\mathrm{e}^{\mp\mathrm{i}\omega_2(t_3-t_1)}\\
&\times\mathrm{e}^{-\mathrm{i}(a+b+c+\mathrm{i}\eta)t}\mathrm{e}^{\mathrm{i}(a-\mathrm{i}\eta)t_1}\mathrm{e}^{\mathrm{i}(b-\mathrm{i}\eta)t_2}\mathrm{e}^{\mathrm{i}(c-\mathrm{i}\eta)t_3}
\end{aligned}
$$

$$
\begin{aligned}
=&\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3 \mathrm{e}^{\pm\mathrm{i}[\omega_1\mp(a+b+c)\mp\mathrm{i}\eta]t}\\
&\times \mathrm{e}^{\pm\mathrm{i}(\omega_2\pm a\mp\mathrm{i}\eta)t_1}\mathrm{e}^{\mp\mathrm{i}(\omega_1\mp b\pm\mathrm{i}\eta)t_2}\mathrm{e}^{\mp\mathrm{i}(\omega_2\mp c\pm\mathrm{i}\eta)t_3}\\
=&\frac{\mp\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times\frac{1}{(\omega_1\mp a\mp c\mp b\pm\mathrm{i}\eta)(\omega_2\mp c\pm\mathrm{i}\eta)(\omega_1+\omega_2\mp c\mp b\pm\mathrm{i}\eta)}\\
=&\frac{-\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\frac{1}{a+c}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times\left(\frac{1}{\omega_1\mp a\mp b\mp c\pm\mathrm{i}\eta}\frac{1}{\omega_1+\omega_2\mp a\mp b\mp 2c\pm\mathrm{i}\eta}\right.\\
&-\frac{1}{\omega_1\mp a\mp b\mp c\pm\mathrm{i}\eta}\frac{1}{\omega_1+\omega_2\mp b\mp c\pm\mathrm{i}\eta}\\
&+\frac{1}{\omega_2\mp c\pm\mathrm{i}\eta}\frac{1}{\omega_1+\omega_2\mp a\mp b\mp 2c\pm\mathrm{i}\eta}\\
&\left.-\frac{1}{\omega_2\mp c\pm\mathrm{i}\eta}\frac{1}{\omega_1+\omega_2\mp b\mp c\pm\mathrm{i}\eta}\right),
\end{aligned}\tag{J.48}
$$

式 (J.48) 的虚部可表示为

$$
\begin{aligned}
&C_{\alpha02}^{(\pm)}C_{\alpha'31}^{(\mp)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3 \mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\Big|_{\mathrm{Im}}\\
=&\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\frac{\pi^2}{a+c}\Big[2f_\alpha^{(\pm)}(\pm a\pm b\pm c) f_{\alpha'}^{(\mp)}(\pm c)\\
&-f_\alpha^{(\pm)}(\pm a\pm b\pm c) f_{\alpha'}^{(\mp)}(\mp a)-f_\alpha^{(\pm)}(\pm b) f_{\alpha'}^{(\mp)}(\pm c)\Big]\\
&-\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times\frac{1}{\omega_1\mp a\mp b\mp c}\frac{1}{\omega_2\mp c}\frac{1}{\omega_1+\omega_2\mp b\mp c},
\end{aligned}\tag{J.49}
$$

同理，式 (J.48) 的实部可表示为

$$
\begin{aligned}
&C_{\alpha02}^{(\pm)}C_{\alpha'31}^{(\mp)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3 \mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\Big|_{\mathrm{Re}}\\
=&\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\frac{\mp\pi}{a+c}f_\alpha^{(\pm)}(\pm a\pm b\pm c)P\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\mp)}(\omega_2)\frac{1}{\omega_2\mp c}
\end{aligned}
$$

$$
\begin{aligned}
&-\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\frac{\mp\pi}{a+c}f_{\alpha}^{(\pm)}(\pm a\pm b\pm c)\,P\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)\,f_{\alpha'}^{(\mp)}(\omega_2)\,\frac{1}{\omega_2\pm a}\\
&+\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\frac{\mp\pi}{a+c}f_{\alpha'}^{(\mp)}(\pm c)\,P\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_{\alpha}(\omega_1)\,f_{\alpha}^{(\pm)}(\omega_1)\,\frac{1}{\omega_1\mp a\mp b\mp c}\\
&-\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{lj}}{(2\pi)^2}\frac{\mp\pi}{a+c}f_{\alpha'}^{(\mp)}(\pm c)\,P\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_{\alpha}(\omega_1)\,f_{\alpha}^{(\pm)}(\omega_1)\,\frac{1}{\omega_1\mp b}\\
&-\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\pm\pi}{a+c}P\int_{-\infty}^{\infty}\mathrm{d}\omega_2 f_{\alpha}^{(\pm)}(-\omega_2\pm b\pm c)\,g_{\alpha'}(\omega_2)\,f_{\alpha'}^{(\mp)}(\omega_2)\,\frac{1}{\omega_2\pm a}\\
&-\frac{\Gamma_{\alpha\sigma}^{ik}\Gamma_{\alpha'\sigma}^{jl}}{(2\pi)^2}\frac{\mp\pi}{a+c}P\int_{-\infty}^{\infty}\mathrm{d}\omega_2 f_{\alpha}^{(\pm)}(-\omega_2\pm b\pm c)\,g_{\alpha'}(\omega_2)\,f_{\alpha'}^{(\mp)}(\omega_2)\,\frac{1}{\omega_2\mp c}.
\end{aligned}
\tag{J.50}
$$

对式 (J.25) 求关于时间 $t_1$，$t_2$ 和 $t_3$ 的积分可得

$$
\begin{aligned}
&C_{\alpha03}^{(\pm)}C_{\alpha'12}^{(\pm)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\\
=&\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_{\alpha}(\omega_1)\,f_{\alpha}^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)\,f_{\alpha'}^{(\pm)}(\omega_2)\\
&\times\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\pm\mathrm{i}\omega_1(t-t_3)}\mathrm{e}^{\pm\mathrm{i}\omega_2(t_1-t_2)}\\
&\times\mathrm{e}^{-\mathrm{i}(a+b+c+\mathrm{i}\eta)t}\mathrm{e}^{\mathrm{i}(a-\mathrm{i}\eta)t_1}\mathrm{e}^{\mathrm{i}(b-\mathrm{i}\eta)t_2}\mathrm{e}^{\mathrm{i}(c-\mathrm{i}\eta)t_3}\\
=&\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_{\alpha}(\omega_1)\,f_{\alpha}^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)\,f_{\alpha'}^{(\pm)}(\omega_2)\\
&\times\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\pm\mathrm{i}[\omega_1\mp(a+b+c)\mp\mathrm{i}\eta]t}\\
&\times\mathrm{e}^{\pm\mathrm{i}(\omega_2\pm a\mp\mathrm{i}\eta)t_1}\mathrm{e}^{\mp\mathrm{i}(\omega_2\mp b\pm\mathrm{i}\eta)t_2}\mathrm{e}^{\mp\mathrm{i}(\omega_1\mp c\pm\mathrm{i}\eta)t_3}\\
=&\frac{\mp\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\lim_{\eta\to0^+}\frac{\displaystyle\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_{\alpha}(\omega_1)\,f_{\alpha}^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)\,f_{\alpha'}^{(\pm)}(\omega_2)}{(\omega_1\mp a\mp c\mp b\pm\mathrm{i}\eta)(\omega_1\mp c\pm\mathrm{i}\eta)(\omega_1+\omega_2\mp c\mp b\pm\mathrm{i}\eta)},
\end{aligned}
\tag{J.51}
$$

式 (J.51) 的实部和虚部可分别表示为

$$
\begin{aligned}
&C_{\alpha03}^{(\pm)}C_{\alpha'12}^{(\pm)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\Big|_{\mathrm{Re}}\\
=&\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_{\alpha}(\omega_1)\,f_{\alpha}^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)\,f_{\alpha'}^{(\pm)}(\omega_2)
\end{aligned}
$$

$$
\begin{aligned}
&\times \frac{\mp\pi}{a+b}\left[\frac{\delta\left(\omega_1 \mp a \mp c \mp b\right)}{\omega_1+\omega_2 \mp c \mp b}+\frac{\delta\left(\omega_1+\omega_2 \mp c \mp b\right)}{\omega_1 \mp a \mp c \mp b}\right.\\
&\left.-\frac{\delta\left(\omega_1 \mp c\right)}{\omega_1+\omega_2 \mp c \mp b}-\frac{\delta\left(\omega_1+\omega_2 \mp c \mp b\right)}{\omega_1 \mp c}\right]\\
=&\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\frac{\mp\pi}{a+b}f_\alpha^{(\pm)}\left(\pm a \pm c \pm b\right)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}\left(\omega_2\right) f_{\alpha'}^{(\pm)}\left(\omega_2\right)\frac{1}{\omega_2 \pm a}\\
&-\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\frac{\mp\pi}{a+b}f_\alpha^{(\pm)}\left(\pm c\right)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}\left(\omega_2\right) f_{\alpha'}^{(\pm)}\left(\omega_2\right)\frac{1}{\omega_2 \mp b}\\
&+\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\frac{\pm\pi}{a+b}\int_{-\infty}^{\infty}\mathrm{d}\omega_2 f_\alpha^{(\pm)}\left(-\omega_2 \pm c \pm b\right) g_{\alpha'}\left(\omega_2\right) f_{\alpha'}^{(\pm)}\left(\omega_2\right)\frac{1}{\omega_2 \pm a}\\
&-\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\frac{\pm\pi}{a+b}\int_{-\infty}^{\infty}\mathrm{d}\omega_2 f_\alpha^{(\pm)}\left(-\omega_2 \pm c \pm b\right) g_{\alpha'}\left(\omega_2\right) f_{\alpha'}^{(\pm)}\left(\omega_2\right)\frac{1}{\omega_2 \mp b},
\end{aligned}\tag{J.52}
$$

$$
\begin{aligned}
&C_{\alpha 03}^{(\pm)}C_{\alpha' 12}^{(\pm)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\Big|_{\mathrm{Im}}\\
=&\frac{-\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha\left(\omega_1\right) f_\alpha^{(\pm)}\left(\omega_1\right)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}\left(\omega_2\right) f_{\alpha'}^{(\pm)}\left(\omega_2\right)\\
&\times\frac{1}{a+b}\left[-\pi^2\delta\left(\omega_1 \mp a \mp c \mp b\right)\delta\left(\omega_1+\omega_2 \mp c \mp b\right)\right.\\
&+\pi^2\delta\left(\omega_1 \mp c\right)\delta\left(\omega_1+\omega_2 \mp c \mp b\right)\\
&\left.+\frac{1}{\omega_1 \mp a \mp c \mp b}\frac{1}{\omega_1+\omega_2 \mp c \mp b}-\frac{1}{\omega_1 \mp c}\frac{1}{\omega_1+\omega_2 \mp c \mp b}\right]\\
=&\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\frac{\pi^2}{a+b}\left[f_\alpha^{(\pm)}\left(\pm a \pm c \pm b\right) f_{\alpha'}^{(\pm)}\left(\mp a\right)-f_\alpha^{(\pm)}\left(\pm c\right) f_{\alpha'}^{(\pm)}\left(\pm b\right)\right]\\
&\mp\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha\left(\omega_1\right) f_\alpha^{(\pm)}\left(\omega_1\right)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}\left(\omega_2\right) f_{\alpha'}^{(\pm)}\left(\omega_2\right)\\
&\times\frac{1}{\omega_1 \mp a \mp c \mp b}\frac{1}{\omega_1 \mp c}\frac{1}{\omega_1+\omega_2 \mp c \mp b}.
\end{aligned}\tag{J.53}
$$

对式 (J.26) 求关于时间 $t_1$，$t_2$ 和 $t_3$ 的积分可得

$$
\begin{aligned}
&C_{\alpha 03}^{(\pm)}C_{\alpha' 12}^{(\mp)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\\
=&\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha\left(\omega_1\right) f_\alpha^{(\pm)}\left(\omega_1\right)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}\left(\omega_2\right) f_{\alpha'}^{(\mp)}\left(\omega_2\right)
\end{aligned}
$$

$$
\begin{aligned}
&\times\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\pm\mathrm{i}\omega_1(t-t_3)}\mathrm{e}^{\mp\mathrm{i}\omega_2(t_1-t_2)}\\
&\times\mathrm{e}^{-\mathrm{i}(a+b+c+\mathrm{i}\eta)t}\mathrm{e}^{\mathrm{i}(a-\mathrm{i}\eta)t_1}\mathrm{e}^{\mathrm{i}(b-\mathrm{i}\eta)t_2}\mathrm{e}^{\mathrm{i}(c-\mathrm{i}\eta)t_3}\\
=&\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{\pm\mathrm{i}[\omega_1\mp(a+b+c)\mp\mathrm{i}\eta]t}\\
&\times\mathrm{e}^{\mp\mathrm{i}(\omega_2\mp a\pm\mathrm{i}\eta)t_1}\mathrm{e}^{\pm\mathrm{i}(\omega_2\pm b\mp\mathrm{i}\eta)t_2}\mathrm{e}^{\mp\mathrm{i}(\omega_1\mp c\pm\mathrm{i}\eta)t_3}\\
=&\frac{\mp\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times\frac{1}{(\omega_1\mp a\mp c\mp b\pm\mathrm{i}\eta)(\omega_1\mp c\pm\mathrm{i}\eta)(\omega_1-\omega_2\mp c\mp b\pm\mathrm{i}\eta)}\\
=&\frac{-\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times\frac{1}{a+b}\left(\frac{1}{\omega_1\mp a\mp c\mp b\pm\mathrm{i}\eta}\frac{1}{\omega_1-\omega_2\mp c\mp b\pm\mathrm{i}\eta}\right.\\
&\left.-\frac{1}{\omega_1\mp c\pm\mathrm{i}\eta}\frac{1}{\omega_1-\omega_2\mp c\mp b\pm\mathrm{i}\eta}\right),
\end{aligned}\tag{J.54}
$$

式 (J.54) 的虚部可表示为

$$
\begin{aligned}
&C_{\alpha03}^{(\pm)}C_{\alpha'12}^{(\mp)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\Big|_{\mathrm{Im}}\\
=&\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\frac{\pi^2}{a+b}f_\alpha^{(\pm)}(\pm a\pm c\pm b)f_{\alpha'}^{(\mp)}(\pm a)\\
&-\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\frac{\pi^2}{a+b}f_\alpha^{(\pm)}(\pm c)f_{\alpha'}^{(\mp)}(\mp b)\\
&\mp\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times\frac{1}{\omega_1\mp a\mp c\mp b}\frac{1}{\omega_1\mp c}\frac{1}{\omega_1-\omega_2\mp c\mp b},
\end{aligned}\tag{J.55}
$$

式 (J.54) 的实部可表示为

$$
\begin{aligned}
&C_{\alpha 03}^{(\pm)} C_{\alpha' 12}^{(\mp)} \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{-\mathrm{i}(a+b+c)t} \mathrm{e}^{\mathrm{i}at_1} \mathrm{e}^{\mathrm{i}bt_2} \mathrm{e}^{\mathrm{i}ct_3} \Big|_{\mathrm{Re}} \\
=&\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2} \int_{-\infty}^{\infty} \mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\mp)}(\omega_2) \\
&\times \frac{\mp\pi}{a+b} \left[ \frac{\delta(\omega_1 \mp a \mp c \mp b)}{\omega_1 - \omega_2 \mp c \mp b} + \frac{\delta(\omega_1 - \omega_2 \mp c \mp b)}{\omega_1 \mp a \mp c \mp b} \right. \\
&\left. - \frac{\delta(\omega_1 \mp c)}{\omega_1 - \omega_2 \mp c \mp b} - \frac{\delta(\omega_1 - \omega_2 \mp c \mp b)}{\omega_1 \mp c} \right] \\
=&\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2} \frac{\pm\pi}{a+b} f_\alpha^{(\pm)}(\pm a \pm c \pm b) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\mp)}(\omega_2) \frac{1}{\omega_2 \mp a} \\
&- \frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2} \frac{\pm\pi}{a+b} f_\alpha^{(\pm)}(\pm c) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\mp)}(\omega_2) \frac{1}{\omega_2 \pm b} \\
&+ \frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2} \frac{\mp\pi}{a+b} f_\alpha^{(\pm)}(\omega_2 \pm c \pm b) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\mp)}(\omega_2) \frac{1}{\omega_2 \mp a} \\
&- \frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2} \frac{\mp\pi}{a+b} f_\alpha^{(\pm)}(\omega_2 \pm c \pm b) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\mp)}(\omega_2) \frac{1}{\omega_2 \pm b}.
\end{aligned} \tag{J.56}
$$

对式 (J.27) 求关于时间 $t_1$，$t_2$ 和 $t_3$ 的积分可得

$$
\begin{aligned}
&C_{\alpha 03}^{(\pm)} C_{\alpha' 21}^{(\pm)} \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{-\mathrm{i}(a+b+c)t} \mathrm{e}^{\mathrm{i}at_1} \mathrm{e}^{\mathrm{i}bt_2} \mathrm{e}^{\mathrm{i}ct_3} \\
=&\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2} \lim_{\eta\to 0^+} \int_{-\infty}^{\infty} \mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\pm)}(\omega_2) \\
&\times \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{\pm\mathrm{i}\omega_1(t-t_3)} \mathrm{e}^{\pm\mathrm{i}\omega_2(t_2-t_1)} \\
&\times \mathrm{e}^{-\mathrm{i}(a+b+c+\mathrm{i}\eta)t} \mathrm{e}^{\mathrm{i}(a-\mathrm{i}\eta)t_1} \mathrm{e}^{\mathrm{i}(b-\mathrm{i}\eta)t_2} \mathrm{e}^{\mathrm{i}(c-\mathrm{i}\eta)t_3} \\
=&\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2} \lim_{\eta\to 0^+} \int_{-\infty}^{\infty} \mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\pm)}(\omega_2) \\
&\times \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{\pm\mathrm{i}(\omega_1 \mp (a+b+c) \mp \mathrm{i}\eta)t} \\
&\times \mathrm{e}^{\mp\mathrm{i}(\omega_2 \mp a \pm \mathrm{i}\eta)t_1} \mathrm{e}^{\pm\mathrm{i}(\omega_2 \pm b \mp \mathrm{i}\eta)t_2} \mathrm{e}^{\mp\mathrm{i}(\omega_1 \mp c \pm \mathrm{i}\eta)t_3} \\
=&\frac{\mp\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2} \lim_{\eta\to 0^+} \int_{-\infty}^{\infty} \mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\pm)}(\omega_2)
\end{aligned}
$$

$$\times \frac{1}{(\omega_1 \mp a \mp c \mp b \pm \mathrm{i}\eta)(\omega_1 \mp c \pm \mathrm{i}\eta)(\omega_1 - \omega_2 \mp c \mp b \pm \mathrm{i}\eta)}$$

$$= \frac{-\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2} \lim_{\eta\to 0^+} \int_{-\infty}^{\infty} \mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\pm)}(\omega_2)$$

$$\times \frac{1}{a+b}\left(\frac{1}{\omega_1 \mp a \mp c \mp b \pm \mathrm{i}\eta} - \frac{1}{\omega_1 \mp c \pm \mathrm{i}\eta}\right)\frac{1}{\omega_1 - \omega_2 \mp c \mp b \pm \mathrm{i}\eta}, \quad \text{(J.57)}$$

式 (J.57) 的实部和虚部可分别表示为

$$C_{\alpha 03}^{(\pm)} C_{\alpha' 21}^{(\pm)} \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{-\mathrm{i}(a+b+c)t} \mathrm{e}^{\mathrm{i}at_1} \mathrm{e}^{\mathrm{i}bt_2} \mathrm{e}^{\mathrm{i}ct_3}\Big|_{\mathrm{Re}}$$

$$= \frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2} \lim_{\eta\to 0^+} \int_{-\infty}^{\infty} \mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\pm)}(\omega_2)$$

$$\times \frac{1}{a+b}\mathrm{Im}\left(\frac{1}{\omega_1 \mp a \mp c \mp b \pm \mathrm{i}\eta} - \frac{1}{\omega_1 \mp c \pm \mathrm{i}\eta}\right)\frac{1}{\omega_1 - \omega_2 \mp c \mp b \pm \mathrm{i}\eta}$$

$$= \frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2} \int_{-\infty}^{\infty} \mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\pm)}(\omega_2)$$

$$\times \frac{\mp\pi}{a+b}\left[\frac{\delta(\omega_1 \mp a \mp c \mp b)}{\omega_1 - \omega_2 \mp c \mp b} + \frac{\delta(\omega_1 - \omega_2 \mp c \mp b)}{\omega_1 \mp a \mp c \mp b}\right.$$

$$\left. - \frac{\delta(\omega_1 \mp c)}{\omega_1 - \omega_2 \mp c \mp b} - \frac{\delta(\omega_1 - \omega_2 \mp c \mp b)}{\omega_1 \mp c}\right]$$

$$= \frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2} \frac{\pm\pi}{a+b} f_\alpha^{(\pm)}(\pm a \pm c \pm b) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\pm)}(\omega_2) \frac{1}{\omega_2 \mp a}$$

$$- \frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2} \frac{\pm\pi}{a+b} f_\alpha^{(\pm)}(\pm c) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\pm)}(\omega_2) \frac{1}{\omega_2 \pm b}$$

$$+ \frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2} \frac{\mp\pi}{a+b} f_\alpha^{(\pm)}(\omega_2 \pm c \pm b) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\pm)}(\omega_2) \frac{1}{\omega_2 \mp a}$$

$$- \frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2} \frac{\mp\pi}{a+b} f_\alpha^{(\pm)}(\omega_2 \pm c \pm b) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\pm)}(\omega_2) \frac{1}{\omega_2 \pm b}, \quad \text{(J.58)}$$

$$C_{\alpha 03}^{(\pm)} C_{\alpha' 21}^{(\pm)} \int_{-\infty}^{t} \mathrm{d}t_1 \int_{-\infty}^{t_1} \mathrm{d}t_2 \int_{-\infty}^{t_2} \mathrm{d}t_3 \mathrm{e}^{-\mathrm{i}(a+b+c)t} \mathrm{e}^{\mathrm{i}at_1} \mathrm{e}^{\mathrm{i}bt_2} \mathrm{e}^{\mathrm{i}ct_3}\Big|_{\mathrm{Im}}$$

$$= -\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2} \lim_{\eta\to 0^+} \int_{-\infty}^{\infty} \mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1) \int_{-\infty}^{\infty} \mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\pm)}(\omega_2)$$

$$\times \frac{1}{a+b}\mathrm{Re}\left(\frac{1}{\omega_1 \mp a \mp c \mp b \pm \mathrm{i}\eta} - \frac{1}{\omega_1 \mp c \pm \mathrm{i}\eta}\right)\frac{1}{\omega_1 - \omega_2 \mp c \mp b \pm \mathrm{i}\eta}$$

$$= \frac{\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2} \frac{\pi^2}{a+b}\left[f_\alpha^{(\pm)}(\pm a \pm c \pm b) f_{\alpha'}^{(\pm)}(\pm a) - f_\alpha^{(\pm)}(\pm c) f_{\alpha'}^{(\pm)}(\mp b)\right]$$

$$
\begin{aligned}
&\mp \frac{\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{jk}}{(2\pi)^2}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\pm)}(\omega_2)\\
&\times \frac{1}{\omega_1\mp a\mp c\mp b}\frac{1}{\omega_1\mp c}\frac{1}{\omega_1-\omega_2\mp c\mp b}.
\end{aligned}
\tag{J.59}
$$

对式 (J.28) 求关于时间 $t_1$，$t_2$ 和 $t_3$ 的积分可得

$$
\begin{aligned}
&C_{\alpha03}^{(\pm)}C_{\alpha'21}^{(\mp)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3 \mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\\
=&\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3 \mathrm{e}^{\pm\mathrm{i}\omega_1(t-t_3)}\mathrm{e}^{\mp\mathrm{i}\omega_2(t_2-t_1)}\\
&\times \mathrm{e}^{-\mathrm{i}(a+b+c+\mathrm{i}\eta)t}\mathrm{e}^{\mathrm{i}(a-\mathrm{i}\eta)t_1}\mathrm{e}^{\mathrm{i}(b-\mathrm{i}\eta)t_2}\mathrm{e}^{\mathrm{i}(c-\mathrm{i}\eta)t_3}\\
=&\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3 \mathrm{e}^{\pm\mathrm{i}[\omega_1\mp(a+b+c)\mp\mathrm{i}\eta]t}\\
&\times \mathrm{e}^{\pm\mathrm{i}(\omega_2\pm a\mp\mathrm{i}\eta)t_1}\mathrm{e}^{\mp\mathrm{i}(\omega_2\mp b\pm\mathrm{i}\eta)t_2}\mathrm{e}^{\mp\mathrm{i}(\omega_1\mp c\pm\mathrm{i}\eta)t_3}\\
=&\frac{\mp\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times\frac{1}{(\omega_1\mp a\mp c\mp b\pm\mathrm{i}\eta)(\omega_1\mp c\pm\mathrm{i}\eta)(\omega_1+\omega_2\mp c\mp b\pm\mathrm{i}\eta)}\\
=&\frac{-\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times\frac{1}{a+b}\left(\frac{1}{\omega_1\mp a\mp c\mp b\pm\mathrm{i}\eta}-\frac{1}{\omega_1\mp c\pm\mathrm{i}\eta}\right)\frac{1}{\omega_1+\omega_2\mp c\mp b\pm\mathrm{i}\eta},
\end{aligned}
\tag{J.60}
$$

式 (J.60) 的虚部可表示为

$$
\begin{aligned}
&C_{\alpha03}^{(\pm)}C_{\alpha'21}^{(\mp)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3 \mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}at_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\Big|_{\mathrm{Im}}\\
=&-\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2}\mathrm{Re}\lim_{\eta\to0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times\frac{1}{a+b}\left(\frac{1}{\omega_1\mp a\mp c\mp b\pm\mathrm{i}\eta}-\frac{1}{\omega_1\mp c\pm\mathrm{i}\eta}\right)\frac{1}{\omega_1+\omega_2\mp c\mp b\pm\mathrm{i}\eta}\\
=&\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2}\frac{\pi^2}{a+b}\left[f_\alpha^{(\pm)}(\pm a\pm c\pm b) f_{\alpha'}^{(\mp)}(\mp a)-f_\alpha^{(\pm)}(\pm c) f_{\alpha'}^{(\mp)}(\pm b)\right]\\
&\mp\frac{\mathrm{i}\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1) f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2) f_{\alpha'}^{(\mp)}(\omega_2)
\end{aligned}
$$

$$\times \frac{1}{\omega_1 \mp a \mp c \mp b}\frac{1}{\omega_1 \mp c}\frac{1}{\omega_1+\omega_2 \mp c \mp b}, \tag{J.61}$$

同理，式 (J.60) 的实部可表示为

$$\begin{aligned}
&C_{\alpha 03}^{(\pm)}C_{\alpha' 21}^{(\mp)}\int_{-\infty}^{t}\mathrm{d}t_1\int_{-\infty}^{t_1}\mathrm{d}t_2\int_{-\infty}^{t_2}\mathrm{d}t_3\mathrm{e}^{-\mathrm{i}(a+b+c)t}\mathrm{e}^{\mathrm{i}ta_1}\mathrm{e}^{\mathrm{i}bt_2}\mathrm{e}^{\mathrm{i}ct_3}\Big|_{\mathrm{Re}}\\
=&\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2}\mathrm{Im}\lim_{\eta\to 0^+}\int_{-\infty}^{\infty}\mathrm{d}\omega_1 g_\alpha(\omega_1)f_\alpha^{(\pm)}(\omega_1)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\mp)}(\omega_2)\\
&\times\frac{1}{a+b}\left(\frac{1}{\omega_1\mp a\mp c\mp b\pm\mathrm{i}\eta}-\frac{1}{\omega_1\mp c\pm\mathrm{i}\eta}\right)\frac{1}{\omega_1+\omega_2\mp c\mp b\pm\mathrm{i}\eta}\\
=&\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2}\frac{\mp\pi}{a+b}f_\alpha^{(\pm)}(\pm a\pm c\pm b)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\mp)}(\omega_2)\frac{1}{\omega_2\pm a}\\
&-\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2}\frac{\mp\pi}{a+b}f_\alpha^{(\pm)}(\pm c)\int_{-\infty}^{\infty}\mathrm{d}\omega_2 g_{\alpha'}(\omega_2)f_{\alpha'}^{(\mp)}(\omega_2)\frac{1}{\omega_2\mp b}\\
&+\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2}\frac{\pm\pi}{a+b}\int_{-\infty}^{\infty}\mathrm{d}\omega_2 f_\alpha^{(\pm)}(-\omega_2\pm c\pm b)g_{\alpha'}(\omega_2)f_{\alpha'}^{(\mp)}(\omega_2)\frac{1}{\omega_2\pm a}\\
&-\frac{\Gamma_{\alpha\sigma}^{il}\Gamma_{\alpha'\sigma}^{kj}}{(2\pi)^2}\frac{\pm\pi}{a+b}\int_{-\infty}^{\infty}\mathrm{d}\omega_2 f_\alpha^{(\pm)}(-\omega_2\pm c\pm b)g_{\alpha'}(\omega_2)f_{\alpha'}^{(\mp)}(\omega_2)\frac{1}{\omega_2\mp b}.
\end{aligned} \tag{J.62}$$

# 附录 K　计算共隧穿过程中矩阵元实部的 2 类积分

在本附录中，给出在共隧穿过程中计算开放量子系统的约化密度矩阵矩阵元的实部涉及的如下两个积分：

$$P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)f_\alpha(\omega_2+b+c)f_{\alpha'}(\omega_2)}{(\omega_2-a)(\omega_2+c)}, \tag{K.1}$$

$$P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)f_\alpha(-\omega_2+b+c)f_{\alpha'}(\omega_2)}{(\omega_2+a)(\omega_2-c)}, \tag{K.2}$$

其中

$$g_{\alpha'}(\omega)=\frac{W^2}{(\omega-\mu_{\alpha'})^2+W^2}. \tag{K.3}$$

对于式 (K.1)，可将其重新表示为

$$\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)f_\alpha(\omega_2+b+c)f_{\alpha'}(\omega_2)}{(\omega_2-a)(\omega_2+c)}\\
=&\frac{1}{a+c}P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)f_\alpha(\omega_2+b+c)f_{\alpha'}(\omega_2)}{\omega_2-a}\\
&-\frac{1}{a+c}P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)f_\alpha(\omega_2+b+c)f_{\alpha'}(\omega_2)}{\omega_2+c},
\end{aligned} \tag{K.4}$$

下面，利用留数定理计算式 (K.4) 的右边第一项，即

$$
\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}\left(\omega_2\right)f_{\alpha}\left(\omega_2+b+c\right)f_{\alpha'}\left(\omega_2\right)}{\omega_2-a}\\
=&P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}\left(\omega_2\right)f_{\alpha'}\left(\omega_2+b+c-\mu_\alpha+\mu_{\alpha'}\right)f_{\alpha'}\left(\omega_2\right)}{\omega_2-a},
\end{aligned}
\tag{K.5}
$$

其中

$$
\begin{aligned}
f_\alpha\left(\omega_2+b+c\right)&=\frac{1}{\mathrm{e}^{\beta\left(\omega_2+b+c-\mu_\alpha\right)}}=\frac{1}{\mathrm{e}^{\beta\left(\omega_2+b+c-\mu_\alpha+\mu_{\alpha'}-\mu_{\alpha'}\right)}}\\
&=f_{\alpha'}\left(\omega_2+b+c-\mu_\alpha+\mu_{\alpha'}\right).
\end{aligned}
\tag{K.6}
$$

为方便计算，令 $x=\beta\left(\omega_2-\mu_{\alpha'}\right)$ 和 $\beta=1/\left(k_{\mathrm{B}}T\right)$，则有

$$
\beta\left(\omega_2+b+c-\mu_\alpha\right)=x+\beta\mu_{\alpha'}+\beta\left(b+c-\mu_\alpha\right)=x-x_0,
\tag{K.7}
$$

其中

$$
x_0=-\beta\left(b+c-\mu_\alpha+\mu_{\alpha'}\right).
\tag{K.8}
$$

同理可得

$$
\omega_2-a=\frac{x-x_1}{\beta},\quad x_1=\beta\left(a-\mu_{\alpha'}\right),
\tag{K.9}
$$

$$
\omega_2-\mu_{\alpha'}-\mathrm{i}W=\frac{x-x_2}{\beta},\quad x_2=\mathrm{i}\beta W,
\tag{K.10}
$$

$$
\omega_2-\mu_{\alpha'}+\mathrm{i}W=\frac{x-x_3}{\beta},\quad x_3=-\mathrm{i}\beta W,
\tag{K.11}
$$

利用式 (K.7)~ 式 (K.11)，可将式 (K.5) 表示为

$$
\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}\left(\omega_2\right)f_{\alpha}\left(\omega_2+b+c\right)f_{\alpha'}\left(\omega_2\right)}{\omega_2-a}\\
=&\left(\beta W\right)^2P\int_{-\infty}^{\infty}\mathrm{d}x\frac{1}{\mathrm{e}^x+1}\frac{1}{\mathrm{e}^{x-x_0}+1}\frac{1}{x-x_1}\frac{1}{x-x_2}\frac{1}{x-x_3}.
\end{aligned}
\tag{K.12}
$$

为计算式 (K.12) 的主值积分，将其被积函数写为

$$
f\left(z\right)=\left(\beta W\right)^2\frac{1}{1+\mathrm{e}^z}\frac{1}{1+\mathrm{e}^{z-x_0}}\frac{1}{z-x_1}\frac{1}{z-x_2}\frac{1}{z-x_3},
\tag{K.13}
$$

其奇点可以表示为

$$
\left\{
\begin{array}{ll}
z_{n,1}=\mathrm{i}\left(2n+1\right)\pi, & n=0,\pm1,\pm2,\cdots\\
z_{n,2}=\mathrm{i}\left(2n+1\right)\pi+x_0, & n=0,\pm1,\pm2,\cdots\\
z_1=x_1 & \\
z_2=x_2 & \\
z_3=x_3 &
\end{array}
\right.,
\tag{K.14}
$$

其中，$z_{n,1}$ 是虚轴上的一阶奇点，$z_{n,2}$ 是复平面上的一阶奇点，$z_1$ 是实轴上的一阶奇点，$z_2$ 是正虚轴上的一阶奇点，$z_3$ 是负虚轴上的一阶奇点. 积分路径选择为，除奇点 $z_1$ 外的实轴部分和在上半平面内以原点为圆心，半径为 $R$ 的半圆组成的围道，如图 A.1 所示. 由留数定理可知

$$\begin{aligned}&\oint_C f(z)\mathrm{d}z\\ =&2\pi\mathrm{i}\sum_{n\geqslant 0}\mathrm{Res}\left[f\left(z\right),z_{n,1}\right]+2\pi\mathrm{i}\sum_{n\geqslant 0}\mathrm{Res}\left[f\left(z\right),z_{n,2}\right]+2\pi\mathrm{i}\mathrm{Res}\left[f\left(z\right),z_2\right],\end{aligned} \tag{K.15}$$

其中

$$\mathrm{Res}\left[f\left(z\right),z_{n,1}\right]=\frac{1}{\mathrm{e}^{-x_0}-1}\left(\frac{1}{z_{n,1}-x_1}-\frac{1}{2}\frac{1}{z_{n,1}-x_2}-\frac{1}{2}\frac{1}{z_{n,1}+x_2}\right), \tag{K.16}$$

$$\begin{aligned}&\mathrm{Res}\left[f\left(z\right),z_{n,2}\right]\\ =&\frac{1}{\mathrm{e}^{x_0}-1}\left(\frac{1}{z_{n,1}+x_0-x_1}-\frac{1}{2}\frac{1}{z_{n,1}+x_0-x_2}-\frac{1}{2}\frac{1}{z_{n,1}+x_0+x_2}\right),\end{aligned} \tag{K.17}$$

$$\mathrm{Res}\left[f\left(z\right),z_2\right]=-\frac{1}{2}\frac{1}{\mathrm{e}^{x_2}+1}\frac{1}{\mathrm{e}^{x_2-x_0}+1}, \tag{K.18}$$

这里，上面三式计算中已经使用了宽带近似，即 $W\gg \mathrm{Max}\{\varepsilon,\mu_\alpha,k_\mathrm{B}T\}$. 将式 (K.16)∼ 式 (K.18) 代入式 (K.15) 可得

$$\begin{aligned}&\oint_C f(z)\mathrm{d}z\\ =&\frac{2\pi i}{\mathrm{e}^{-x_0}-1}\left(\frac{1}{z_{n,1}-x_1}-\frac{1}{2}\frac{1}{z_{n,1}-x_2}-\frac{1}{2}\frac{1}{z_{n,1}+x_2}\right)-\pi\mathrm{i}\frac{1}{\mathrm{e}^{x_2}+1}\frac{1}{\mathrm{e}^{x_2-x_0}+1}\\ &+\frac{2\pi\mathrm{i}}{\mathrm{e}^{x_0}-1}\left(\frac{1}{z_{n,1}+x_0-x_1}-\frac{1}{2}\frac{1}{z_{n,1}+x_0-x_2}-\frac{1}{2}\frac{1}{z_{n,1}+x_0+x_2}\right).\end{aligned} \tag{K.19}$$

由于当 $|z|\to\infty$ 时，积分

$$\lim_{|z|\to\infty}zf\left(z\right)=\left(\beta W\right)^2\lim_{|z|\to\infty}z\frac{1}{1+\mathrm{e}^z}\frac{1}{1+\mathrm{e}^{z-x_0}}\frac{1}{z-x_1}\frac{1}{z-x_2}\frac{1}{z-x_3}=0, \tag{K.20}$$

因而有

$$\int_{C_R}f\left(z\right)\mathrm{d}z=0. \tag{K.21}$$

此外，在宽带近似下，积分

$$\int_{C_r}f\left(z\right)\mathrm{d}z=-\mathrm{i}\pi\mathrm{Res}\left[f\left(z\right),x_1\right]=-\mathrm{i}\pi\frac{1}{\mathrm{e}^{x_1}+1}\frac{1}{\mathrm{e}^{x_1-x_0}+1}\ . \tag{K.22}$$

当 $R\to\infty$，且 $r\to 0$ 时，$f(z)$ 的主值积分可表示为

$$\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}x\frac{1}{1+\mathrm{e}^{z}}\frac{1}{1+\mathrm{e}^{z-x_0}}\frac{1}{z-x_1}\frac{1}{z-x_2}\frac{1}{z-x_3}\\
=&\oint_{C}f(z)\mathrm{d}z-\int_{C_R}f(z)\,\mathrm{d}z-\int_{C_r}f(z)\,\mathrm{d}z\\
=&\frac{2\pi\mathrm{i}}{\mathrm{e}^{-x_0}-1}\left(\frac{1}{z_{n,1}-x_1}-\frac{1}{2}\frac{1}{z_{n,1}-x_2}-\frac{1}{2}\frac{1}{z_{n,1}+x_2}\right)\\
&+\frac{2\pi\mathrm{i}}{\mathrm{e}^{x_0}-1}\left(\frac{1}{z_{n,1}+x_0-x_1}-\frac{1}{2}\frac{1}{z_{n,1}+x_0-x_2}-\frac{1}{2}\frac{1}{z_{n,1}+x_0+x_2}\right)\\
&-\pi\mathrm{i}\frac{1}{\mathrm{e}^{x_2}+1}\frac{1}{\mathrm{e}^{x_2-x_0}+1}+\mathrm{i}\pi\frac{1}{\mathrm{e}^{x_1}+1}\frac{1}{\mathrm{e}^{x_1-x_0}+1},
\end{aligned}\tag{K.23}$$

即

$$\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)\,f_{\alpha}(\omega_2+b+c)\,f_{\alpha'}(\omega_2)}{\omega_2-a}\\
=&\frac{2\pi\mathrm{i}}{\mathrm{e}^{-x_0}-1}\left(\frac{1}{z_{n,1}-x_{1,a}}-\frac{1}{2}\frac{1}{z_{n,1}-x_2}-\frac{1}{2}\frac{1}{z_{n,1}+x_2}\right)\\
&+\frac{2\pi\mathrm{i}}{\mathrm{e}^{x_0}-1}\left(\frac{1}{z_{n,1}+x_0-x_{1,a}}-\frac{1}{2}\frac{1}{z_{n,1}+x_0-x_2}-\frac{1}{2}\frac{1}{z_{n,1}+x_0+x_2}\right)\\
&-\pi\mathrm{i}\frac{1}{\mathrm{e}^{x_2}+1}\frac{1}{\mathrm{e}^{x_2-x_0}+1}+\mathrm{i}\pi\frac{1}{\mathrm{e}^{x_{1,a}}+1}\frac{1}{\mathrm{e}^{x_{1,a}-x_0}+1},
\end{aligned}\tag{K.24}$$

其中，$x_{1,a}=\beta\,(a-\mu_{\alpha'})$. 同理，令 $x_{1,c}=-\beta\,(c+\mu_{\alpha'})$，可得

$$\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)\,f_{\alpha}(\omega_2+b+c)\,f_{\alpha'}(\omega_2)}{\omega_2+c}\\
=&\frac{2\pi\mathrm{i}}{\mathrm{e}^{-x_0}-1}\left(\frac{1}{z_{n,1}-x_{1,c}}-\frac{1}{2}\frac{1}{z_{n,1}-x_2}-\frac{1}{2}\frac{1}{z_{n,1}+x_2}\right)\\
&+\frac{2\pi\mathrm{i}}{\mathrm{e}^{x_0}-1}\left(\frac{1}{z_{n,1}+x_0-x_{1,c}}-\frac{1}{2}\frac{1}{z_{n,1}+x_0-x_2}-\frac{1}{2}\frac{1}{z_{n,1}+x_0+x_2}\right)\\
&-\pi\mathrm{i}\frac{1}{\mathrm{e}^{x_2}+1}\frac{1}{\mathrm{e}^{x_2-x_0}+1}+\mathrm{i}\pi\frac{1}{\mathrm{e}^{x_{1,c}}+1}\frac{1}{\mathrm{e}^{x_{1,c}-x_0}+1},
\end{aligned}\tag{K.25}$$

将式 (K.24) 和 (K.25) 代入式 (K.4) 可得

$$\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)\,f_{\alpha}(\omega_2+b+c)\,f_{\alpha'}(\omega_2)}{(\omega_2-a)\,(\omega_2+c)}\\
=&\frac{1}{a+c}\frac{2\pi\mathrm{i}}{\mathrm{e}^{-x_0}-1}\left(\frac{1}{z_{n,1}-x_{1,a}}-\frac{1}{z_{n,1}-x_{1,c}}\right)\\
&+\frac{1}{a+c}\frac{2\pi\mathrm{i}}{\mathrm{e}^{x_0}-1}\left(\frac{1}{z_{n,1}+x_0-x_{1,a}}-\frac{1}{z_{n,1}+x_0-x_{1,c}}\right)
\end{aligned}$$

$$+\frac{\mathrm{i}\pi}{a+c}\left(\frac{1}{\mathrm{e}^{x_{1,a}}+1}\frac{1}{\mathrm{e}^{x_{1,a}-x_0}+1}-\frac{1}{\mathrm{e}^{x_{1,c}}+1}\frac{1}{\mathrm{e}^{x_{1,c}-x_0}+1}\right), \tag{K.26}$$

由双伽马函数的性质

$$\Psi(z)=\lim_{n\to\infty}\left(\ln n-\sum_{k=0}^{\infty}\frac{1}{k+z}\right), \tag{K.27}$$

可将式 (K.26) 简化为

$$\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)\,f_\alpha(\omega_2+b+c)\,f_{\alpha'}(\omega_2)}{(\omega_2-a)(\omega_2+c)}\\
=&\frac{1}{a+c}\frac{1}{\mathrm{e}^{-x_0}-1}\left[-\Psi\left(\frac{1}{2}+\mathrm{i}\frac{x_{1,a}}{2\pi}\right)+\Psi\left(\frac{1}{2}+\mathrm{i}\frac{x_{1,c}}{2\pi}\right)\right]\\
&+\frac{1}{a+c}\frac{1}{\mathrm{e}^{x_0}-1}\left[-\Psi\left(\frac{1}{2}+\mathrm{i}\frac{x_{1,a}-x_0}{2\pi}\right)+\Psi\left(\frac{1}{2}+\mathrm{i}\frac{x_{1,c}-x_0}{2\pi}\right)\right]\\
&+\frac{\mathrm{i}\pi}{a+c}\left(\frac{1}{\mathrm{e}^{x_{1,a}}+1}\frac{1}{\mathrm{e}^{x_{1,a}-x_0}+1}-\frac{1}{\mathrm{e}^{x_{1,c}}+1}\frac{1}{\mathrm{e}^{x_{1,c}-x_0}+1}\right),
\end{aligned} \tag{K.28}$$

利用双伽马函数的性质

$$\Psi\left(\frac{1}{2}+\mathrm{i}\frac{x_1}{2\pi}\right)=\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{x_1}{2\pi}\right)-\frac{\mathrm{i}\pi}{2}\tanh\left(-\frac{x_1}{2}\right), \tag{K.29}$$

可以将式 (K.28) 重新表示为

$$\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)\,f_\alpha(\omega_2+b+c)\,f_{\alpha'}(\omega_2)}{(\omega_2-a)(\omega_2+c)}\\
=&\frac{1}{a+c}\frac{1}{\mathrm{e}^{-x_0}-1}\left[-\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{x_{1,a}}{2\pi}\right)+\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{x_{1,c}}{2\pi}\right)\right]\\
&+\frac{1}{a+c}\frac{1}{\mathrm{e}^{x_0}-1}\left[-\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{x_{1,a}-x_0}{2\pi}\right)+\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{x_{1,c}-x_0}{2\pi}\right)\right]\\
&+\frac{1}{2}\frac{\mathrm{i}\pi}{a+c}\left[\frac{2}{\mathrm{e}^{x_{1,a}}+1}\frac{1}{\mathrm{e}^{x_{1,a}-x_0}+1}+\frac{1}{\mathrm{e}^{-x_0}-1}\tanh\left(-\frac{x_{1,a}}{2}\right)\right.\\
&\left.+\frac{1}{\mathrm{e}^{x_0}-1}\tanh\left(\frac{x_0-x_{1,a}}{2}\right)\right]\\
&-\frac{1}{2}\frac{\mathrm{i}\pi}{a+c}\left[\frac{2}{\mathrm{e}^{x_{1,c}}+1}\frac{1}{\mathrm{e}^{x_{1,c}-x_0}+1}+\frac{1}{\mathrm{e}^{-x_0}-1}\tanh\left(-\frac{x_{1,c}}{2}\right)\right.\\
&\left.+\frac{1}{\mathrm{e}^{x_0}-1}\tanh\left(\frac{x_0-x_{1,c}}{2}\right)\right],
\end{aligned} \tag{K.30}$$

由于

$$
\begin{aligned}
&2\frac{1}{\mathrm{e}^{x_1}+1}\frac{1}{\mathrm{e}^{x_1-x_0}+1}+\frac{1}{\mathrm{e}^{-x_0}-1}\tanh\left(-\frac{x_1}{2}\right)+\frac{1}{\mathrm{e}^{x_0}-1}\tanh\left(\frac{x_0-x_1}{2}\right)\\
=&2\frac{1}{\mathrm{e}^{x_1}+1}\frac{1}{\mathrm{e}^{x_1-x_0}+1}-\frac{\mathrm{e}^{x_0}}{\mathrm{e}^{x_0}-1}\frac{1-\mathrm{e}^{x_1}}{1+\mathrm{e}^{x_1}}+\frac{1}{\mathrm{e}^{x_0}-1}\frac{1-\mathrm{e}^{x_1-x_0}}{1+\mathrm{e}^{x_1-x_0}}\\
=&2\frac{1}{\mathrm{e}^{x_1}+1}\left(\frac{1}{\mathrm{e}^{x_1-x_0}+1}-1\right)-2\frac{1}{\mathrm{e}^{x_0}-1}\left(\frac{1}{1+\mathrm{e}^{x_1}}-\frac{1}{1+\mathrm{e}^{x_1-x_0}}\right)+1\\
=&2\frac{1}{\mathrm{e}^{x_1}+1}\frac{-\mathrm{e}^{x_1-x_0}}{\mathrm{e}^{x_1-x_0}+1}-2\frac{1}{\mathrm{e}^{x_0}-1}\frac{\mathrm{e}^{x_1-x_0}-\mathrm{e}^{x_1}}{(1+\mathrm{e}^{x_1})(1+\mathrm{e}^{x_1-x_0})}+1\\
=&2\frac{1}{\mathrm{e}^{x_1}+1}\frac{\mathrm{e}^{x_1}-\mathrm{e}^{x_1-x_0}-\mathrm{e}^{x_1}+\mathrm{e}^{x_1-x_0}}{\mathrm{e}^{x_0}-1}+1=1,
\end{aligned}
\tag{K.31}
$$

因而，式 (K.30) 可进一步简化为

$$
\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)f_\alpha(\omega_2+b+c)f_{\alpha'}(\omega_2)}{(\omega_2-a)(\omega_2+c)}\\
=&\frac{1}{a+c}\frac{1}{\mathrm{e}^{-x_0}-1}\left[-\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{x_{1,a}}{2\pi}\right)+\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{x_{1,c}}{2\pi}\right)\right]\\
&+\frac{1}{a+c}\frac{1}{\mathrm{e}^{x_0}-1}\left[-\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{x_{1,a}-x_0}{2\pi}\right)+\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{x_{1,c}-x_0}{2\pi}\right)\right],
\end{aligned}
\tag{K.32}
$$

将式 (K.8)、$x_{1,a}=\beta(a-\mu_{\alpha'})$ 以及 $x_{1,c}=-\beta(c+\mu_{\alpha'})$ 代入上式可得

$$
\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)f_\alpha(\omega_2+b+c)f_{\alpha'}(\omega_2)}{(\omega_2-a)(\omega_2+c)}\\
=&-\frac{1}{a+c}\frac{1}{\mathrm{e}^{\frac{b+c-\mu_\alpha+\mu_{\alpha'}}{k_\mathrm{B}T}}-1}\left[\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{a-\mu_{\alpha'}}{2\pi k_\mathrm{B}T}\right)-\mathrm{Re}\Psi\left(\frac{1}{2}-\mathrm{i}\frac{c+\mu_{\alpha'}}{2\pi k_\mathrm{B}T}\right)\right]\\
&+\frac{1}{a+c}\frac{\mathrm{e}^{\frac{b+c-\mu_\alpha+\mu_{\alpha'}}{k_\mathrm{B}T}}}{\mathrm{e}^{\frac{b+c-\mu_\alpha+\mu_{\alpha'}}{k_\mathrm{B}T}}-1}\left[\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{a+b+c-\mu_\alpha}{2\pi k_\mathrm{B}T}\right)\right.\\
&\left.-\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{b-\mu_\alpha}{2\pi k_\mathrm{B}T}\right)\right].
\end{aligned}
\tag{K.33}
$$

下面计算式 (K.2) 的主值积分，为方便计算，将被积函数中的两个费米分布函数的乘积重新写为

$$
\begin{aligned}
&f_\alpha(-\omega_2+b+c)f_{\alpha'}(\omega_2)\\
=&\frac{1}{\mathrm{e}^{-\omega_2+b+c-\mu_\alpha}+1}\frac{1}{\mathrm{e}^{\omega_2-\mu_{\alpha'}}+1}=\frac{\mathrm{e}^{\omega_2-b-c+\mu_\alpha}}{\mathrm{e}^{\omega_2-b-c+\mu_\alpha}+1}\frac{1}{\mathrm{e}^{\omega_2-\mu_{\alpha'}}+1}\\
=&\left(\frac{1}{\mathrm{e}^{\omega_2-b-c+\mu_\alpha}+1}-\frac{1}{\mathrm{e}^{\omega_2-\mu_{\alpha'}}+1}\right)\frac{\mathrm{e}^{\omega_2-b-c+\mu_\alpha}}{\mathrm{e}^{\omega_2-\mu_{\alpha'}}-\mathrm{e}^{\omega_2-b-c+\mu_\alpha}}
\end{aligned}
$$

$$
\begin{aligned}
&= \left[f_{\alpha'}\left(\omega_2 - b - c + \mu_\alpha + \mu_{\alpha'}\right) - f_{\alpha'}\left(\omega_2\right)\right] \frac{1}{\mathrm{e}^{b+c-\mu_\alpha-\mu_{\alpha'}} - 1} \\
&= \left[f_{\alpha'}\left(\omega_2 - b - c + \mu_\alpha + \mu_{\alpha'}\right) - f_{\alpha'}\left(\omega_2\right)\right] b_{\alpha'}\left(b + c - \mu_\alpha\right),
\end{aligned} \tag{K.34}
$$

其中

$$
b_{\alpha'}\left(b+c-\mu_\alpha\right) = \frac{1}{\mathrm{e}^{b+c-\mu_\alpha-\mu_{\alpha'}} - 1}. \tag{K.35}
$$

因此，式 (K.2) 的主值积分可以重写为

$$
\begin{aligned}
& P\int_{-\infty}^{\infty} \mathrm{d}\omega_2 \frac{g_{\alpha'}\left(\omega_2\right) f_\alpha\left(-\omega_2 + b + c\right) f_{\alpha'}\left(\omega_2\right)}{\left(\omega_2 + a\right)\left(\omega_2 - c\right)} \\
=& b_{\alpha'}\left(b+c-\mu_\alpha\right) P\int_{-\infty}^{\infty} \mathrm{d}\omega_2 \frac{g_{\alpha'}\left(\omega_2\right) f_{\alpha'}\left(\omega_2 - b - c + \mu_\alpha + \mu_{\alpha'}\right)}{\left(\omega_2 + a\right)\left(\omega_2 - c\right)} \\
& - b_{\alpha'}\left(b+c-\mu_\alpha\right) P\int_{-\infty}^{\infty} \mathrm{d}\omega_2 \frac{g_{\alpha'}\left(\omega_2\right) f_{\alpha'}\left(\omega_2\right)}{\left(\omega_2 + a\right)\left(\omega_2 - c\right)} \\
=& -\frac{b_{\alpha'}\left(b+c-\mu_\alpha\right)}{a+c} P\int_{-\infty}^{\infty} \mathrm{d}\omega_2 \frac{g_{\alpha'}\left(\omega_2\right) f_{\alpha'}\left(\omega_2 - b - c + \mu_\alpha + \mu_{\alpha'}\right)}{\omega_2 + a} \\
& + \frac{b_{\alpha'}\left(b+c-\mu_\alpha\right)}{a+c} P\int_{-\infty}^{\infty} \mathrm{d}\omega_2 \frac{g_{\alpha'}\left(\omega_2\right) f_{\alpha'}\left(\omega_2\right)}{\omega_2 + a} \\
& + \frac{b_{\alpha'}\left(b+c-\mu_\alpha\right)}{a+c} P\int_{-\infty}^{\infty} \mathrm{d}\omega_2 \frac{g_{\alpha'}\left(\omega_2\right) f_{\alpha'}\left(\omega_2 - b - c + \mu_\alpha + \mu_{\alpha'}\right)}{\omega_2 - c} \\
& - \frac{b_{\alpha'}\left(b+c-\mu_\alpha\right)}{a+c} P\int_{-\infty}^{\infty} \mathrm{d}\omega_2 \frac{g_{\alpha'}\left(\omega_2\right) f_{\alpha'}\left(\omega_2\right)}{\omega_2 - c},
\end{aligned} \tag{K.36}
$$

将式 (K.36) 右边的第一项和第三项作如下变量替换：$\omega = \omega_2 - b - c + \mu_\alpha + \mu_{\alpha'}$ 可得

$$
\begin{aligned}
& P\int_{-\infty}^{\infty} \mathrm{d}\omega_2 \frac{g_{\alpha'}\left(\omega_2\right) f_\alpha\left(-\omega_2 + b + c\right) f_{\alpha'}\left(\omega_2\right)}{\left(\omega_2 + a\right)\left(\omega_2 - c\right)} \\
=& -\frac{b_{\alpha'}\left(b+c-\mu_\alpha\right)}{a+c} P\int_{-\infty}^{\infty} \mathrm{d}\omega_2 \frac{g_{\alpha'}\left(\omega_2\right) f_{\alpha'}\left(\omega_2\right)}{\omega_2 - \left(-a - b - c + \mu_\alpha + \mu_{\alpha'}\right)} \\
& + \frac{b_{\alpha'}\left(b+c-\mu_\alpha\right)}{a+c} P\int_{-\infty}^{\infty} \mathrm{d}\omega_2 \frac{g_{\alpha'}\left(\omega_2\right) f_{\alpha'}\left(\omega_2\right)}{\omega_2 - (-a)} \\
& + \frac{b_{\alpha'}\left(b+c-\mu_\alpha\right)}{a+c} P\int_{-\infty}^{\infty} \mathrm{d}\omega_2 \frac{g_{\alpha'}\left(\omega_2\right) f_{\alpha'}\left(\omega_2\right)}{\omega_2 - \left(-b + \mu_\alpha + \mu_{\alpha'}\right)} \\
& - \frac{b_{\alpha'}\left(b+c-\mu_\alpha\right)}{a+c} P\int_{-\infty}^{\infty} \mathrm{d}\omega_2 \frac{g_{\alpha'}\left(\omega_2\right) f_{\alpha'}\left(\omega_2\right)}{\omega_2 - c},
\end{aligned} \tag{K.37}
$$

利用式 (A.34)

$$
P\int_{-\infty}^{\infty} \mathrm{d}\omega \frac{g_{\alpha'}(\omega) f_{\alpha'}(\omega)}{\omega - \Delta} = \mathrm{Re}\Psi\left(\frac{1}{2} + \mathrm{i}\frac{\Delta - \mu_{\alpha'}}{2\pi k_{\mathrm{B}} T}\right) - \ln\frac{W}{2\pi k_{\mathrm{B}} T}, \tag{K.38}
$$

可将式 (K.36) 表示为

$$
\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)\,f_\alpha(-\omega_2+b+c)\,f_{\alpha'}(\omega_2)}{(\omega_2+a)(\omega_2-c)}\\
=&-\frac{b_{\alpha'}(b+c-\mu_\alpha)}{a+c}\mathrm{Re}\Psi\left(\frac{1}{2}-\mathrm{i}\frac{a+b+c-\mu_\alpha}{2\pi k_{\mathrm{B}}T}\right)\\
&+\frac{b_{\alpha'}(b+c-\mu_\alpha)}{a+c}\mathrm{Re}\Psi\left(\frac{1}{2}-\mathrm{i}\frac{a+\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)\\
&+\frac{b_{\alpha'}(b+c-\mu_\alpha)}{a+c}\mathrm{Re}\Psi\left(\frac{1}{2}-\mathrm{i}\frac{b-\mu_\alpha}{2\pi k_{\mathrm{B}}T}\right)\\
&-\frac{b_{\alpha'}(b+c-\mu_\alpha)}{a+c}\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right).
\end{aligned}\tag{K.39}
$$

# 附录 L　计算共隧穿过程中矩阵元虚部的 4 类积分

在本附录中，给出在共隧穿过程中计算开放量子系统的约化密度矩阵矩阵元的虚部涉及的如下四个积分：

$$P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_\alpha(\omega_1)\,f_\alpha(\omega_1)\,g_{\alpha'}(\omega_2)\,f_{\alpha'}(\omega_2)}{(\omega_1-a-c-b)(\omega_2-c)(\omega_1+\omega_2-c-b)},\tag{L.1}$$

$$P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_\alpha(\omega_1)\,f_\alpha(\omega_1)\,g_{\alpha'}(\omega_2)\,f_{\alpha'}(\omega_2)}{(\omega_1-a-c-b)(\omega_2+c)(\omega_1-\omega_2-c-b)},\tag{L.2}$$

$$P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_\alpha(\omega_1)\,f_\alpha(\omega_1)\,g_{\alpha'}(\omega_2)\,f_{\alpha'}(\omega_2)}{(\omega_1-a-c-b)(\omega_1-c)(\omega_1+\omega_2-c-b)},\tag{L.3}$$

$$P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_\alpha(\omega_1)\,f_\alpha(\omega_1)\,g_{\alpha'}(\omega_2)\,f_{\alpha'}(\omega_2)}{(\omega_1-a-c-b)(\omega_1-c)(\omega_1-\omega_2-b-c)}.\tag{L.4}$$

为了计算上面四个主值积分，首先计算下面两个积分：

$$\mathrm{Re}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\Psi\left(\frac{1}{2}+\mathrm{i}\frac{c-\omega_1-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)\frac{g_{\alpha i}(\omega_1)\,f_{\alpha i}(\omega_1)}{\omega_1-a},\tag{L.5}$$

$$\mathrm{Re}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\Psi\left(\frac{1}{2}+\mathrm{i}\frac{\omega_1-c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)\frac{g_{\alpha i}(\omega_1)\,f_{\alpha i}(\omega_1)}{\omega_1-a}.\tag{L.6}$$

其中

$$g_\alpha(\omega)=\frac{W^2}{(\omega-\mu_\alpha)^2+W^2}.\tag{L.7}$$

为方便计算，令 $x=\beta(\omega_1-\mu_\alpha)$ 和 $\beta=1/(k_{\mathrm{B}}T)$，则有

$$\frac{\beta(c-\omega_1-\mu_{\alpha'})}{2\pi}=-\frac{x-x_0}{2\pi},\tag{L.8}$$

其中

$$x_0 = \beta\left(c - \mu_\alpha - \mu_{\alpha'}\right). \tag{L.9}$$

同理可得

$$\omega_1 - a = \frac{x - x_1}{\beta}, \quad x_1 = \beta\left(a - \mu_\alpha\right), \tag{L.10}$$

$$\omega_1 - \mu_{\alpha'} - \mathrm{i}W = \frac{x - x_2}{\beta}, \quad x_2 = \mathrm{i}\beta W, \tag{L.11}$$

$$\omega_1 - \mu_{\alpha'} + \mathrm{i}W = \frac{x - x_3}{\beta}, \quad x_3 = -\mathrm{i}\beta W. \tag{L.12}$$

利用上面的式 (L.8)∼ 式 (L.12)，可将式 (L.5) 表示为

$$\begin{aligned}&\mathrm{Re}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\Psi\left(\frac{1}{2}+\mathrm{i}\frac{c-\omega_1-\mu_{\alpha j}}{2\pi k_{\mathrm{B}}T}\right)\frac{g_{\alpha i}\left(\omega_1\right)f_{\alpha i}\left(\omega_1\right)}{\omega_1-a}\\&=\left(\beta W\right)^2\mathrm{Re}P\int_{-\infty}^{\infty}\mathrm{d}x\Psi\left(\frac{1}{2}-\mathrm{i}\frac{x-x_0}{2\pi}\right)\frac{1}{\mathrm{e}^x+1}\frac{1}{x-x_1}\frac{1}{x-x_2}\frac{1}{x-x_3},\end{aligned} \tag{L.13}$$

为计算式 (L.13) 的主值积分，将其被积函数写为

$$f\left(z\right) = \left(\beta W\right)^2\Psi\left(\frac{1}{2}-\mathrm{i}\frac{z-x_0}{2\pi}\right)\frac{1}{1+\mathrm{e}^z}\frac{1}{z-x_1}\frac{1}{z-x_2}\frac{1}{z-x_3}, \tag{L.14}$$

其奇点可以表示为

$$\begin{cases} z_{n,1} = x_0 - \mathrm{i}\left(2n+1\right)\pi, & n = 0, 1, 2, \cdots \\ z_{n,2} = \mathrm{i}\left(2n+1\right)\pi, & n = 0, \pm 1, \pm 2, \cdots \\ z_1 = x_1 & \\ z_2 = x_2 & \\ z_3 = x_3 & \end{cases}, \tag{L.15}$$

其中，$z_{n,1}$ 是下半复平面的一阶奇点，$z_{n,2}$ 是虚轴上的一阶奇点，$z_1$ 是实轴上的一阶奇点，$z_2$ 是正虚轴上的一阶奇点，$z_3$ 是负虚轴上的一阶奇点. 积分路径选择为，除奇点 $z_1$ 外的实轴部分和在上半平面内以原点为圆心，半径为 $R$ 的半圆组成的围道，如图 A.1 所示. 由留数定理可知

$$\oint_C f(z)\mathrm{d}z = 2\pi\mathrm{i}\sum_{n\geqslant 0}\mathrm{Res}\left[f\left(z\right), z_{n,2}\right] + 2\pi\mathrm{i}\mathrm{Res}\left[f\left(z\right), z_2\right], \tag{L.16}$$

其中

$$2\pi\mathrm{i}\mathrm{Res}\left[f\left(z\right), z_{n,2}\right]$$

$$=-\pi\mathrm{i}\sum_{n\geqslant 0}\Psi\left(\frac{1}{2}-\mathrm{i}\frac{z_{n,2}-x_0}{2\pi}\right)\left(\frac{2}{z_{n,2}-x_1}-\frac{1}{z_{n,2}+x_2}-\frac{1}{z_{n,2}-x_2}\right), \tag{L.17}$$

$$2\pi\mathrm{i}\mathrm{Res}\left[f\left(z\right),z_2\right]=-\pi\mathrm{i}\Psi\left(\frac{1}{2}-\mathrm{i}\frac{x_2-x_0}{2\pi}\right)\frac{1}{\mathrm{e}^{x_2}+1}, \tag{L.18}$$

这里，上面两式计算中已经使用了宽带近似，即 $W\gg\max\{\varepsilon,\mu_\alpha,k_\mathrm{B}T\}$. 将式 (L.17) 和 (L.18) 代入式 (L.16) 可得

$$\begin{aligned}&\oint_C f(z)\mathrm{d}z\\&=-\pi\mathrm{i}\sum_{n\geqslant 0}\Psi\left(\frac{1}{2}-\mathrm{i}\frac{z_{n,2}-x_0}{2\pi}\right)\left(\frac{2}{z_{n,2}-x_1}-\frac{1}{z_{n,2}+x_2}-\frac{1}{z_{n,2}-x_2}\right)\\&\quad-\pi\mathrm{i}\Psi\left(\frac{1}{2}-\mathrm{i}\frac{x_2-x_0}{2\pi}\right)\frac{1}{\mathrm{e}^{x_2}+1}.\end{aligned} \tag{L.19}$$

由于当 $|z|\to\infty$ 时，积分

$$\begin{aligned}\lim_{|z|\to\infty}zf\left(z\right)=&\left(\beta W\right)^2\lim_{|z|\to\infty}z\Psi\left(\frac{1}{2}-\mathrm{i}\frac{z-x_0}{2\pi}\right)\frac{1}{1+\mathrm{e}^z}\frac{1}{z-x_1}\frac{1}{z-x_2}\frac{1}{z-x_3}\\=&0,\end{aligned} \tag{L.20}$$

因而有

$$\int_{C_R}f\left(z\right)\mathrm{d}z=0. \tag{L.21}$$

此外，在宽带近似下，积分

$$\int_{C_r}f\left(z\right)\mathrm{d}z=-\mathrm{i}\pi\mathrm{Res}\left[f\left(z\right),x_1\right]=-\mathrm{i}\pi\Psi\left(\frac{1}{2}-\mathrm{i}\frac{x_1-x_0}{2\pi}\right)\frac{1}{\mathrm{e}^{x_1}+1}\ . \tag{L.22}$$

当 $R\to\infty$，且 $r\to 0$ 时，$f\left(z\right)$ 的主值积分可表示为

$$\begin{aligned}&\left(\beta W\right)^2P\int_{-\infty}^{\infty}\mathrm{d}x\Psi\left(\frac{1}{2}-\mathrm{i}\frac{z-x_0}{2\pi}\right)\frac{1}{1+\mathrm{e}^z}\frac{1}{z-x_1}\frac{1}{z-x_2}\frac{1}{z-x_3}\\=&\oint_C f(z)\mathrm{d}z-\int_{C_R}f\left(z\right)\mathrm{d}z-\int_{C_r}f\left(z\right)\mathrm{d}z\\=&-\pi\mathrm{i}\sum_{n\geqslant 0}\Psi\left(\frac{1}{2}-\mathrm{i}\frac{z_{n,2}-x_0}{2\pi}\right)\left(\frac{2}{z_{n,2}-x_1}-\frac{1}{z_{n,2}+x_2}-\frac{1}{z_{n,2}-x_2}\right)\\&-\pi\mathrm{i}\Psi\left(\frac{1}{2}-\mathrm{i}\frac{x_2-x_0}{2\pi}\right)\frac{1}{\mathrm{e}^{x_2}+1}+\mathrm{i}\pi\Psi\left(\frac{1}{2}-\mathrm{i}\frac{x_1-x_0}{2\pi}\right)\frac{1}{\mathrm{e}^{x_1}+1},\end{aligned} \tag{L.23}$$

即

$$\left(\beta W\right)^2\mathrm{Re}P\int_{-\infty}^{\infty}\mathrm{d}x\Psi\left(\frac{1}{2}-\mathrm{i}\frac{z-x_0}{2\pi}\right)\frac{1}{1+\mathrm{e}^z}\frac{1}{z-x_1}\frac{1}{z-x_2}\frac{1}{z-x_3}$$

$$
\begin{aligned}
&=\pi \mathrm{Im}\sum_{n\geqslant 0}\Psi\left(\frac{1}{2}-\mathrm{i}\frac{z_{n,2}-x_0}{2\pi}\right)\left(\frac{2}{z_{n,2}-x_1}-\frac{1}{z_{n,2}+x_2}-\frac{1}{z_{n,2}-x_2}\right)\\
&\quad+\pi \mathrm{Im}\Psi\left(\frac{1}{2}-\mathrm{i}\frac{x_2-x_0}{2\pi}\right)\frac{1}{\mathrm{e}^{x_2}+1}-\pi \mathrm{Im}\Psi\left(\frac{1}{2}-\mathrm{i}\frac{x_1-x_0}{2\pi}\right)\frac{1}{\mathrm{e}^{x_1}+1},
\end{aligned}\tag{L.24}
$$

将式 (L.9)～ 式 (L.11) 以及式 (L.15) 代入式 (L.24) 可得

$$
\begin{aligned}
&\mathrm{Re}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\Psi\left(\frac{1}{2}+\mathrm{i}\frac{-\omega_1+c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)\frac{g_{\alpha i}\left(\omega_1\right)f_{\alpha i}\left(\omega_1\right)}{\omega_1-a}\\
&=\pi \mathrm{Im}\sum_{n\geqslant 0}\Psi\left(n+1+\mathrm{i}\frac{-\mu_\alpha+c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)\left[\frac{2}{\mathrm{i}\pi\left(2n+1\right)-\left(a-\mu_\alpha\right)/\left(k_{\mathrm{B}}T\right)}\right.\\
&\quad\left.-\frac{1}{\mathrm{i}\pi\left(2n+1\right)+\mathrm{i}W/\left(k_{\mathrm{B}}T\right)}-\frac{1}{\mathrm{i}\pi\left(2n+1\right)-\mathrm{i}W/(k_{\mathrm{B}}T)}\right]\\
&\quad+\pi \mathrm{Im}\Psi\left(\frac{1}{2}+\frac{W}{2\pi k_{\mathrm{B}}T}+\mathrm{i}\frac{-\mu_\alpha+c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)\frac{1}{\mathrm{e}^{\mathrm{i}W/(k_{\mathrm{B}}T)}+1}\\
&\quad-\pi \mathrm{Im}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{-a+c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)\frac{1}{\mathrm{e}^{(a-\mu_\alpha)/(k_{\mathrm{B}}T)}+1},
\end{aligned}\tag{L.25}
$$

利用双伽马函数的性质 $[\Psi\left(z\right)]^*=\Psi\left(z^*\right)$ 可得

$$
\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{\omega_1-c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)=\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{-\omega_1+c+\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right),\tag{L.26}
$$

因此，式 (L.6) 的主值积分可表示为

$$
\begin{aligned}
&\mathrm{Re}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\mathit{\Psi}\left(\frac{1}{2}+\mathrm{i}\frac{-\omega_1+c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)\frac{g_{\alpha i}\left(\omega_1\right)f_{\alpha i}\left(\omega_1\right)}{\omega_1-a}\\
&=\pi \mathrm{Im}\sum_{n\geqslant 0}\Psi\left(n+1+\mathrm{i}\frac{-\mu_\alpha+c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)\left[\frac{2}{\mathrm{i}\pi\left(2n+1\right)-\left(a-\mu_\alpha\right)/(k_{\mathrm{B}}T)}\right.\\
&\quad\left.-\frac{1}{\mathrm{i}\pi\left(2n+1\right)+\mathrm{i}W/(k_{\mathrm{B}}T)}-\frac{1}{\mathrm{i}\pi\left(2n+1\right)-\mathrm{i}W/(k_{\mathrm{B}}T)}\right]\\
&\quad+\pi \mathrm{Im}\Psi\left(\frac{1}{2}+\frac{W}{2\pi k_{\mathrm{B}}T}+\mathrm{i}\frac{-\mu_\alpha+c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)\frac{1}{\mathrm{e}^{\mathrm{i}W/(k_{\mathrm{B}}T)}+1}\\
&\quad-\pi \mathrm{Im}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{-a+c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)\frac{1}{\mathrm{e}^{(a-\mu_\alpha)/(k_{\mathrm{B}}T)}+1}.
\end{aligned}\tag{L.27}
$$

下面计算式 (L.1)～ 式 (L.4) 的积分主值，为此，将其被积函数中除费米分布函数 $f_\alpha\left(\omega\right)$ 和态密度函数 $g_\alpha\left(\omega\right)$ 外的部分分别展开为

$$
\begin{aligned}
&\frac{1}{\left(\omega_1-a-c-b\right)\left(\omega_2-c\right)\left(\omega_1+\omega_2-c-b\right)}\\
&=\frac{1}{a+c}\left(\frac{1}{\omega_1-a-c-b}+\frac{1}{\omega_2-c}\right)
\end{aligned}
$$

$$\times\left(\frac{1}{\omega_1+\omega_2-a-b-2c}-\frac{1}{\omega_1+\omega_2-c-b}\right), \tag{L.28}$$

$$\begin{aligned}&\frac{1}{(\omega_1-a-c-b)(\omega_2+c)(\omega_1-\omega_2-c-b)}\\=&\frac{1}{a+c}\left(\frac{1}{\omega_1-a-c-b}-\frac{1}{\omega_2+c}\right)\\&\times\left(\frac{1}{\omega_1-\omega_2-c-b}-\frac{1}{\omega_1-\omega_2-a-b-2c}\right),\end{aligned} \tag{L.29}$$

$$\begin{aligned}&\frac{1}{(\omega_1-a-c-b)(\omega_1-c)(\omega_1+\omega_2-c-b)}\\=&\frac{1}{a+b}\left(\frac{1}{\omega_1-a-c-b}-\frac{1}{\omega_1-c}\right)\frac{1}{\omega_1+\omega_2-c-b},\end{aligned} \tag{L.30}$$

$$\begin{aligned}&\frac{1}{(\omega_1-a-c-b)(\omega_1-c)(\omega_1-\omega_2-b-c)}\\=&\frac{1}{a+b}\left(\frac{1}{\omega_1-a-c-b}-\frac{1}{\omega_1-c}\right)\frac{1}{\omega_1-\omega_2-c-b}.\end{aligned} \tag{L.31}$$

因此，式 (L.1)~ 式 (L.4) 的积分主值可以分别表示为

$$\begin{aligned}&P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_\alpha(\omega_1)f_\alpha(\omega_1)g_{\alpha'}(\omega_2)f_{\alpha'}(\omega_2)}{(\omega_1-a-c-b)(\omega_2-c)(\omega_1+\omega_2-c-b)}\\=&\frac{1}{a+c}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)f_{\alpha'}(\omega_2)}{\omega_2+\omega_1-a-b-2c}\frac{g_\alpha(\omega_1)f_\alpha(\omega_1)}{\omega_1-a-c-b}\\&-\frac{1}{a+c}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)f_{\alpha'}(\omega_2)}{\omega_2+\omega_1-c-b}\frac{g_\alpha(\omega_1)f_\alpha(\omega_1)}{\omega_1-a-c-b}\\&+\frac{1}{a+c}P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\int_{-\infty}^{\infty}\mathrm{d}\omega_1\frac{g_\alpha(\omega_1)f_\alpha(\omega_1)}{\omega_1+\omega_2-a-b-2c}\frac{g_{\alpha'}(\omega_2)f_{\alpha'}(\omega_2)}{\omega_2-c}\\&-\frac{1}{a+c}P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\int_{-\infty}^{\infty}\mathrm{d}\omega_1\frac{g_\alpha(\omega_1)f_\alpha(\omega_1)}{\omega_1+\omega_2-c-b}\frac{g_{\alpha'}(\omega_2)f_{\alpha'}(\omega_2)}{\omega_2-c},\end{aligned} \tag{L.32}$$

$$\begin{aligned}&P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_\alpha(\omega_1)f_\alpha(\omega_1)g_{\alpha'}(\omega_2)f_{\alpha'}(\omega_2)}{(\omega_1-a-c-b)(\omega_2+c)(\omega_1-\omega_2-c-b)}\\=&-\frac{1}{a+c}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)f_{\alpha'}(\omega_2)}{\omega_2-\omega_1+c+b}\frac{g_\alpha(\omega_1)f_\alpha(\omega_1)}{\omega_1-a-c-b}\\&+\frac{1}{a+c}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}(\omega_2)f_{\alpha'}(\omega_2)}{\omega_2-\omega_1+a+b+2c}\frac{g_\alpha(\omega_1)f_\alpha(\omega_1)}{\omega_1-a-c-b}\end{aligned}$$

$$
\begin{aligned}
&-\frac{1}{a+c}P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\int_{-\infty}^{\infty}\mathrm{d}\omega_1\frac{g_\alpha\left(\omega_1\right)f_\alpha\left(\omega_1\right)}{\omega_1-\omega_2-c-b}\frac{g_{\alpha'}\left(\omega_2\right)f_{\alpha'}\left(\omega_2\right)}{\omega_2+c}\\
&+\frac{1}{a+c}P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\int_{-\infty}^{\infty}\mathrm{d}\omega_1\frac{g_\alpha\left(\omega_1\right)f_\alpha\left(\omega_1\right)}{\omega_1-\omega_2-a-b-2c}\frac{g_{\alpha'}\left(\omega_2\right)f_{\alpha'}\left(\omega_2\right)}{\omega_2+c},
\end{aligned}
\tag{L.33}
$$

$$
\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_\alpha\left(\omega_1\right)f_\alpha\left(\omega_1\right)g_{\alpha'}\left(\omega_2\right)f_{\alpha'}\left(\omega_2\right)}{\left(\omega_1-a-c-b\right)\left(\omega_1-c\right)\left(\omega_1+\omega_2-c-b\right)}\\
=&\frac{1}{a+b}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}\left(\omega_2\right)f_{\alpha'}\left(\omega_2\right)}{\omega_2+\omega_1-c-b}\frac{g_\alpha\left(\omega_1\right)f_\alpha\left(\omega_1\right)}{\omega_1-a-c-b}\\
&-\frac{1}{a+b}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}\left(\omega_2\right)f_{\alpha'}\left(\omega_2\right)}{\omega_2+\omega_1-c-b}\frac{g_\alpha\left(\omega_1\right)f_\alpha\left(\omega_1\right)}{\omega_1-c},
\end{aligned}
\tag{L.34}
$$

$$
\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_\alpha\left(\omega_1\right)f_\alpha\left(\omega_1\right)g_{\alpha'}\left(\omega_2\right)f_{\alpha'}\left(\omega_2\right)}{\left(\omega_1-a-c-b\right)\left(\omega_1-c\right)\left(\omega_1-\omega_2-b-c\right)}\\
=&-\frac{1}{a+b}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}\left(\omega_2\right)f_{\alpha'}\left(\omega_2\right)}{\omega_2-\omega_1+c+b}\frac{g_\alpha\left(\omega_1\right)f_\alpha\left(\omega_1\right)}{\omega_1-a-c-b}\\
&+\frac{1}{a+b}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_{\alpha'}\left(\omega_2\right)f_{\alpha'}\left(\omega_2\right)}{\omega_2-\omega_1+c+b}\frac{g_\alpha\left(\omega_1\right)f_\alpha\left(\omega_1\right)}{\omega_1-c}.
\end{aligned}
\tag{L.35}
$$

利用式 (A.34)

$$
P\int_{-\infty}^{\infty}\mathrm{d}\omega\frac{g_\alpha\left(\omega\right)f_\alpha\left(\omega\right)}{\omega-\Delta}=\mathrm{Re}\Psi\left(\frac{1}{2}+\mathrm{i}\frac{\Delta-\mu_\alpha}{2\pi k_{\mathrm{B}}T}\right)-\ln\frac{W}{2\pi k_{\mathrm{B}}T},
\tag{L.36}
$$

可将式 (L.32)~ 式 (L.35) 分别表示为

$$
\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_\alpha\left(\omega_1\right)f_\alpha\left(\omega_1\right)g_{\alpha'}\left(\omega_2\right)f_{\alpha'}\left(\omega_2\right)}{\left(\omega_1-a-c-b\right)\left(\omega_2-c\right)\left(\omega_1+\omega_2-c-b\right)}\\
=&\frac{1}{a+c}\mathrm{Re}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\frac{\Psi\left(\dfrac{1}{2}+\mathrm{i}\dfrac{-\omega_1+a+b+2c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)g_\alpha\left(\omega_1\right)f_\alpha\left(\omega_1\right)}{\omega_1-a-c-b}\\
&-\frac{1}{a+c}\mathrm{Re}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\frac{\Psi\left(\dfrac{1}{2}+\mathrm{i}\dfrac{-\omega_1+b+c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)g_\alpha\left(\omega_1\right)f_\alpha\left(\omega_1\right)}{\omega_1-a-c-b}\\
&+\frac{1}{a+c}\mathrm{Re}P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{\Psi\left(\dfrac{1}{2}+\mathrm{i}\dfrac{-\omega_2+a+b+2c-\mu_\alpha}{2\pi k_{\mathrm{B}}T}\right)g_{\alpha'}\left(\omega_2\right)f_{\alpha'}\left(\omega_2\right)}{\omega_2-c}\\
&-\frac{1}{a+c}\mathrm{Re}P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{\Psi\left(\dfrac{1}{2}+\mathrm{i}\dfrac{-\omega_2+b+c-\mu_\alpha}{2\pi k_{\mathrm{B}}T}\right)g_{\alpha'}\left(\omega_2\right)f_{\alpha'}\left(\omega_2\right)}{\omega_2-c},
\end{aligned}
\tag{L.37}
$$

$$
\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_\alpha(\omega_1)\,f_\alpha(\omega_1)\,g_{\alpha'}(\omega_2)\,f_{\alpha'}(\omega_2)}{(\omega_1-a-c-b)\,(\omega_2+c)\,(\omega_1-\omega_2-c-b)}\\
=&-\frac{1}{a+c}\mathrm{Re}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\frac{\Psi\left(\dfrac{1}{2}+\mathrm{i}\dfrac{\omega_1-b-c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)g_\alpha(\omega_1)\,f_\alpha(\omega_1)}{\omega_1-a-c-b}\\
&+\frac{1}{a+c}\mathrm{Re}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\frac{\Psi\left(\dfrac{1}{2}+\mathrm{i}\dfrac{\omega_1-a-b-2c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)g_\alpha(\omega_1)\,f_\alpha(\omega_1)}{\omega_1-a-c-b}\\
&-\frac{1}{a+c}\mathrm{Re}P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{\Psi\left(\dfrac{1}{2}+\mathrm{i}\dfrac{\omega_2+b+c-\mu_{\alpha}}{2\pi k_{\mathrm{B}}T}\right)g_{\alpha'}(\omega_2)\,f_{\alpha'}(\omega_2)}{\omega_2+c}\\
&+\frac{1}{a+c}\mathrm{Re}P\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{\Psi\left(\dfrac{1}{2}+\mathrm{i}\dfrac{\omega_2+a+b+2c-\mu_{\alpha}}{2\pi k_{\mathrm{B}}T}\right)g_{\alpha'}(\omega_2)\,f_{\alpha'}(\omega_2)}{\omega_2+c},
\end{aligned}
\tag{L.38}
$$

$$
\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_\alpha(\omega_1)\,f_\alpha(\omega_1)\,g_{\alpha'}(\omega_2)\,f_{\alpha'}(\omega_2)}{(\omega_1-a-c-b)\,(\omega_1-c)\,(\omega_1+\omega_2-c-b)}\\
=&\frac{1}{a+b}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\frac{\Psi\left(\dfrac{1}{2}+\mathrm{i}\dfrac{-\omega_1+b+c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)g_\alpha(\omega_1)\,f_\alpha(\omega_1)}{\omega_1-a-c-b}\\
&-\frac{1}{a+b}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\frac{\Psi\left(\dfrac{1}{2}+\mathrm{i}\dfrac{-\omega_1+b+c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)g_\alpha(\omega_1)\,f_\alpha(\omega_1)}{\omega_1-c}\\
&+\frac{1}{a+b}\ln\frac{W}{2\pi k_{\mathrm{B}}T}\left[P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\frac{g_\alpha(\omega_1)\,f_\alpha(\omega_1)}{\omega_1-c}\right.\\
&\left.-P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\frac{g_\alpha(\omega_1)\,f_\alpha(\omega_1)}{\omega_1-a-c-b}\right],
\end{aligned}
\tag{L.39}
$$

$$
\begin{aligned}
&P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\int_{-\infty}^{\infty}\mathrm{d}\omega_2\frac{g_\alpha(\omega_1)\,f_\alpha(\omega_1)\,g_{\alpha'}(\omega_2)\,f_{\alpha'}(\omega_2)}{(\omega_1-a-c-b)\,(\omega_1-c)\,(\omega_1-\omega_2-b-c)}\\
=&-\frac{1}{a+b}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\frac{\Psi\left(\dfrac{1}{2}+\mathrm{i}\dfrac{\omega_1-b-c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)g_\alpha(\omega_1)\,f_\alpha(\omega_1)}{\omega_1-a-c-b}\\
&+\frac{1}{a+b}P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\frac{\Psi\left(\dfrac{1}{2}+\mathrm{i}\dfrac{\omega_1-b-c-\mu_{\alpha'}}{2\pi k_{\mathrm{B}}T}\right)g_\alpha(\omega_1)\,f_\alpha(\omega_1)}{\omega_1-c}\\
&+\frac{1}{a+b}\ln\frac{W}{2\pi k_{\mathrm{B}}T}\left[P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\frac{g_\alpha(\omega_1)\,f_\alpha(\omega_1)}{\omega_1-a-c-b}-P\int_{-\infty}^{\infty}\mathrm{d}\omega_1\frac{g_\alpha(\omega_1)\,f_\alpha(\omega_1)}{\omega_1-c}\right].
\end{aligned}
\tag{L.40}
$$

将式 (L.25) 和式 (L.27) 代入式 (L.37)∼ 式 (L.40) 可得式 (L.1)∼ 式 (L.4) 的

积分主值，由于表达式比较长，这里略去.

另外，对于式 (L.1)~ 式 (L.4) 中的费米分布函数为

$$f_{\alpha}\left(\omega_{1}\right) \rightarrow 1-f_{\alpha}\left(\omega_{1}\right), \quad f_{\alpha'}\left(\omega_{2}\right) \rightarrow 1-f_{\alpha'}\left(\omega_{2}\right), \tag{L.41}$$

还需要计算如下两个积分主值：

$$\operatorname{Re} P \int_{-\infty}^{\infty} \mathrm{d} \omega_{2} \Psi\left(\frac{1}{2}+\mathrm{i} \frac{c-\omega_{1}-\mu_{\alpha'}}{2 \pi k_{\mathrm{B}} T}\right) \frac{g_{\alpha}\left(\omega_{1}\right)}{\omega_{1}-a}, \tag{L.42}$$

$$\operatorname{Re} P \int_{-\infty}^{\infty} \mathrm{d} \omega_{2} \Psi\left(\frac{1}{2}+\mathrm{i} \frac{\omega_{1}-c-\mu_{\alpha'}}{2 \pi k_{\mathrm{B}} T}\right) \frac{g_{\alpha}\left(\omega_{1}\right)}{\omega_{1}-a}, \tag{L.43}$$

基于留数定理和双伽马函数的性质，在宽带近似下，式 (L.42) 和式 (L.43) 的主值积分可表示为

$$\begin{aligned}
&\operatorname{Re} P \int_{-\infty}^{\infty} \mathrm{d} \omega_{2} \Psi\left(\frac{1}{2}+\mathrm{i} \frac{c-\omega_{1}-\mu_{\alpha'}}{2 \pi k_{\mathrm{B}} T}\right) \frac{g_{\alpha}\left(\omega_{1}\right)}{\omega_{1}-a} \\
=&\pi \operatorname{Im} \Psi\left(\frac{1}{2}+\frac{W}{2 \pi k_{\mathrm{B}} T}+\mathrm{i} \frac{-\mu_{\alpha}+c-\mu_{\alpha'}}{2 \pi k_{\mathrm{B}} T}\right)-\pi \operatorname{Im} \Psi\left(\frac{1}{2}+\mathrm{i} \frac{-a+c-\mu_{\alpha'}}{2 \pi k_{\mathrm{B}} T}\right),
\end{aligned} \tag{L.44}$$

$$\begin{aligned}
&\operatorname{Re} P \int_{-\infty}^{\infty} \mathrm{d} \omega_{2} \Psi\left(\frac{1}{2}+\mathrm{i} \frac{\omega_{1}-c-\mu_{\alpha'}}{2 \pi k_{\mathrm{B}} T}\right) \frac{g_{\alpha}\left(\omega_{1}\right)}{\omega_{1}-a} \\
=&\operatorname{Re} P \int_{-\infty}^{\infty} \mathrm{d} \omega_{2} \Psi\left(\frac{1}{2}+\mathrm{i} \frac{-\omega_{1}+c+\mu_{\alpha'}}{2 \pi k_{\mathrm{B}} T}\right) \frac{g_{\alpha}\left(\omega_{1}\right)}{\omega_{1}-a} \\
=&\pi \operatorname{Im} \Psi\left(\frac{1}{2}+\frac{W}{2 \pi k_{\mathrm{B}} T}+\mathrm{i} \frac{-\mu_{\alpha}+c+\mu_{\alpha'}}{2 \pi k_{\mathrm{B}} T}\right)-\pi \operatorname{Im} \Psi\left(\frac{1}{2}+\mathrm{i} \frac{-a+c+\mu_{\alpha'}}{2 \pi k_{\mathrm{B}} T}\right).
\end{aligned} \tag{L.45}$$

## 参 考 文 献

[1] 吴崇试. 数学物理方法. 2 版. 北京：北京大学出版社，2003：104.

[2] Timm C. Time-convolutionless master equation for quantum dots: Perturbative expansion to arbitrary order. Phys. Rev. B, 2011, 83: 115416.

[3] Breuer H P, Petruccione F. The Theory of Open Quantum Systems. Oxford: Oxford University Press, 2002: 443, 444.

[4] Flindt C, Novotný T, Braggio A, et al. Counting statistics of transport through Coulomb blockade nanostructures: High-order cumulants and non-Markovian effects. Phys. Rev. B, 2010, 82: 155407.

# 《现代物理基础丛书》已出版书目

（按出版时间排序）

| | | |
|---|---|---|
| 1. 现代声学理论基础 | 马大猷 著 | 2004.03 |
| 2. 物理学家用微分几何（第二版） | 侯伯元，侯伯宇 著 | 2004.08 |
| 3. 数学物理方程及其近似方法 | 程建春 编著 | 2004.08 |
| 4. 计算物理学 | 马文淦 编著 | 2005.05 |
| 5. 相互作用的规范理论（第二版） | 戴元本 著 | 2005.07 |
| 6. 理论力学 | 张建树，等 编著 | 2005.08 |
| 7. 微分几何入门与广义相对论（上册·第二版） | 梁灿彬，周彬 著 | 2006.01 |
| 8. 物理学中的群论（第二版） | 马中骐 著 | 2006.02 |
| 9. 辐射和光场的量子统计 | 曹昌祺 著 | 2006.03 |
| 10. 实验物理中的概率和统计（第二版） | 朱永生 著 | 2006.04 |
| 11. 声学理论与工程应用 | 何 琳 等 编著 | 2006.05 |
| 12. 高等原子分子物理学（第二版） | 徐克尊 著 | 2006.08 |
| 13. 大气声学（第二版） | 杨训仁，陈宇 著 | 2007.06 |
| 14. 输运理论（第二版） | 黄祖洽 著 | 2008.01 |
| 15. 量子统计力学（第二版） | 张先蔚 编著 | 2008.02 |
| 16. 凝聚态物理的格林函数理论 | 王怀玉 著 | 2008.05 |
| 17. 激光光散射谱学 | 张明生 著 | 2008.05 |
| 18. 量子非阿贝尔规范场论 | 曹昌祺 著 | 2008.07 |
| 19. 狭义相对论（第二版） | 刘 辽 等 编著 | 2008.07 |
| 20. 经典黑洞与量子黑洞 | 王永久 著 | 2008.08 |
| 21. 路径积分与量子物理导引 | 侯伯元 等 著 | 2008.09 |
| 22. 量子光学导论 | 谭维翰 著 | 2009.01 |
| 23. 全息干涉计量——原理和方法 | 熊秉衡，李俊昌 编著 | 2009.01 |
| 24. 实验数据多元统计分析 | 朱永生 编著 | 2009.02 |
| 25. 微分几何入门与广义相对论(中册·第二版) | 梁灿彬，周彬 著 | 2009.03 |
| 26. 中子引发轻核反应的统计理论 | 张竞上 著 | 2009.03 |

| | | |
|---|---|---|
| 27. 工程电磁理论 | 张善杰 著 | 2009.08 |
| 28. 微分几何入门与广义相对论(下册·第二版) | 梁灿彬, 周彬 著 | 2009.08 |
| 29. 经典电动力学 | 曹昌祺 著 | 2009.08 |
| 30. 经典宇宙和量子宇宙 | 王永久 著 | 2010.04 |
| 31. 高等结构动力学(第二版) | 李东旭 著 | 2010.09 |
| 32. 粉末衍射法测定晶体结构(第二版·上、下册) | 梁敬魁 编著 | 2011.03 |
| 33. 量子计算与量子信息原理 | Giuliano Benenti 等 著 | |
| ——第一卷：基本概念 | 王文阁, 李保文 译 | 2011.03 |
| 34. 近代晶体学(第二版) | 张克从 著 | 2011.05 |
| 35. 引力理论(上、下册) | 王永久 著 | 2011.06 |
| 36. 低温等离子体 | В. М. 弗尔曼, И. М. 扎什京 编著 | |
| ——等离子体的产生、工艺、问题及前景 | 邱励俭 译 | 2011.06 |
| 37. 量子物理新进展 | 梁九卿，韦联福 著 | 2011.08 |
| 38. 电磁波理论 | 葛德彪，魏 兵 著 | 2011.08 |
| 39. 激光光谱学 | W. 戴姆特瑞德 著 | |
| ——第 1 卷：基础理论 | 姬 扬 译 | 2012.02 |
| 40. 激光光谱学 | W. 戴姆特瑞德 著 | |
| ——第 2 卷：实验技术 | 姬 扬 译 | 2012.03 |
| 41. 量子光学导论(第二版) | 谭维翰 著 | 2012.05 |
| 42. 中子衍射技术及其应用 | 姜传海, 杨传铮 编著 | 2012.06 |
| 43. 凝聚态、电磁学和引力中的多值场论 | H. 克莱纳特 著 | |
| | 姜 颖 译 | 2012.06 |
| 44. 反常统计动力学导论 | 包景东 著 | 2012.06 |
| 45. 实验数据分析(上册) | 朱永生 著 | 2012.06 |
| 46. 实验数据分析(下册) | 朱永生 著 | 2012.06 |
| 47. 有机固体物理 | 解士杰, 等 著 | 2012.09 |
| 48. 磁性物理 | 金汉民 著 | 2013.01 |
| 49. 自旋电子学 | 翟宏如, 等 编著 | 2013.01 |
| 50. 同步辐射光源及其应用(上册) | 麦振洪, 等 著 | 2013.03 |
| 51. 同步辐射光源及其应用(下册) | 麦振洪, 等 著 | 2013.03 |

| | | |
|---|---|---|
| 52．高等量子力学 | 汪克林　著 | 2013.03 |
| 53．量子多体理论与运动模式动力学 | 王顺金　著 | 2013.03 |
| 54．薄膜生长（第二版） | 吴自勤，等　著 | 2013.03 |
| 55．物理学中的数学方法 | 王怀玉　著 | 2013.03 |
| 56．物理学前沿——问题与基础 | 王顺金　著 | 2013.06 |
| 57．弯曲时空量子场论与量子宇宙学 | 刘　辽，黄超光　著 | 2013.10 |
| 58．经典电动力学 | 张锡珍，张焕乔　著 | 2013.10 |
| 59．内应力衍射分析 | 姜传海，杨传铮　编著 | 2013.11 |
| 60．宇宙学基本原理 | 龚云贵　著 | 2013.11 |
| 61．B 介子物理学 | 肖振军　著 | 2013.11 |
| 62．量子场论与重整化导论 | 石康杰，等　编著 | 2014.06 |
| 63．粒子物理导论 | 杜东生，杨茂志　著 | 2015.01 |
| 64．固体量子场论 | 史俊杰，等　著 | 2015.03 |
| 65．物理学中的群论（第三版）——有限群篇 | 马中骐　著 | 2015.03 |
| 66．中子引发轻核反应的统计理论（第二版） | 张竞上　著 | 2015.03 |
| 67．自旋玻璃与消息传递 | 周海军　著 | 2015.06 |
| 68．粒子物理学导论 | 肖振军，吕才典　著 | 2015.07 |
| 69．量子系统的辛算法 | 丁培柱　编著 | 2015.07 |
| 70．原子分子光电离物理及实验 | 汪正民　著 | 2015.08 |
| 71．量子场论 | 李灵峰　著 | 2015.09 |
| 72．原子核结构 | 张锡珍，张焕乔　著 | 2015.10 |
| 73．物理学中的群论（第三版）——李代数篇 | 马中骐　著 | 2015.10 |
| 74．量子场论导论 | 姜志进　编著 | 2015.12 |
| 75．高能物理实验统计分析 | 朱永生　著 | 2016.01 |
| 76．数学物理方程及其近似方法 | 程建春　著 | 2016.06 |
| 77．电弧等离子体炬 | M. F. 朱可夫 等 编著<br>陈明周，邱励俭 译 | 2016.06 |
| 78．现代宇宙学 | Scott Dodelson　著<br>张同杰，于浩然　译 | 2016.08 |
| 79．现代电磁理论基础 | 王长清，李明之　著 | 2017.03 |

| | | |
|---|---|---|
| 80．非平衡态热力学 | 翟玉春　编著 | 2017.04 |
| 81．论理原子结构 | 朱颀人　著 | 2017.04 |
| 82．粒子物理导论（第二版） | 杜东生，杨茂志　著 | 2017.06 |
| 83．正电子散射物理 | 吴奕初，蒋中英，郁伟中　编著 | 2017.09 |
| 84．量子光场的性质与应用 | 孟祥国，王继锁　著 | 2017.12 |
| 85．介观电路的量子理论与量子计算 | 梁宝龙，王继锁　著 | 2018.06 |
| **86．开放量子系统的电子计数统计理论** | **薛海斌　著** | **2018.12** |

(O-7558.31)

科学出版社互联网入口

科学数理分社
电话：(010) 64033515
Email：zhouhan@mail.sciencep.com
销售分类建议：高等物理

www.sciencep.com

ISBN 978-7-03-059914-8

定 价：98.00 元